RESONANT STATE EXPANSION APPLIED TO OPEN

OPTICAL SYSTEMS

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Declaration

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

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Abstract

This thesis presents work that I have done with Egor Muljarov and Wolfgang Langbein in order to extend an existing perturbation theory for open systems describable by a scalar equation to 3D systems which cannot be reduced to effectively lower dimensions. This perturbation theory is called the resonant-state expansion (RSE). The RSE is derived from properties of the dyadic tensor Green's function (GF) of the unperturbed system written in terms of resonant states (RSs). Hence to extend the RSE it was necessary for us to derive this spectral form of the GF in terms of normalised RSs for arbitrary 3D systems. To process the numerical output of the RSE, we develop and evaluated algorithms for error estimation and their reduction by extrapolation.

In the case of planar systems the RSE can be compared with other methods such as the scattering matrix or transfer matrix methods. It is also possible to solve the boundary conditions analytically to provide transcendental equations that can be solved by the Newton-Raphson method. We study these systems for that reason since we can validate the numerical calculations of the RSE by showing the convergence of perturbed solutions to the exact result found from these other methods. We study the planar systems both zero and non-zero in-plane wavevector.

As an intermediate step to a fully 3D perturbation theory for open systems we make an implementation of the RSE in 2D. We use as a basis the analytically known RSs of the infinitely extended homogeneous dielectric cylinder. We find that the unperturbed GF contains a cut in the complex frequency plane, which must be included in the RSE basis for the accuracy of the perturbation theory. Zero frequency longitudinal modes are found to be formal solutions of Maxwell's wave equation which also must be included in the basis for the accuracy of the method. Zero frequency modes occur for systems of all dimensionality when considering the TM modes, modes with electric field component normal to the interfaces.

In the penultimate chapter of this thesis we apply the RSE to fully 3D open systems. We use as a basis the analytically known RSs of the homogeneous dielectric sphere. This advance was non-trivial due to a general mixing of transversal and longitudinal electro-magnetic modes. We compare the performance of the RSE with available commercial electromagnetic solvers. In the case of 3D perturbations, we find that the RSE provides a higher accuracy than the finite element method (FEM) and finite difference in time domain (FDTD) for a given computational effort, demonstrating its potential to supersede presently used methods.

At the end of the penultimate chapter we introduce a local perturbation method for RSE, which is a unique capability of the RSE compared to FEM or FDTD, and allows to calculate small perturbations of a system with a small computational effort.

Publications

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M. B. Doost, W. Langbein, and E. A. Muljarov. Resonant-state expansion applied to two-dimensional open optical systems. Phys. Rev. A 87, 043827 (2013).

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Chapter 1

Introduction

It is in most cases not possible to solve eigenvalue problems analytically. Perturbative methods and various expansions into complete sets of functions are currently being used to solve eigenvalue problems, as we will discuss in Sec. 1.2. At the beginning of my PhD the perturbation method named resonant-state expansion (RSE) allowed for the expansion of the eigenstates of arbitrary electrodynamic systems in terms of sets of analytically known solutions of similar problems differing from the system of interest by some perturbation. However at that time the RSE was only rigorously proven and implemented for systems reducible to a scalar equation. In this thesis I will present work that I have undertaken with my supervisors Egor Muljarov and Wolfgang Langbein to extend the RSE to systems of two and three dimensions.

In this thesis the RSE will be shown to be useful for the calculation of whispering gallery modes in bio-sensors and photonic wave guides. The Lorentzian frequency linewidth of these resonant modes is twice the imaginary part of the complex frequency. The finite linewidths of resonances are typical for open systems and are due to energy leakage from the system to the outside. This leakage can be enhanced by various structural imperfections and scatterers. In particular, when an object is placed inside or in close proximity to the cavity, the resulting modification of the electromagnetic susceptibility perturbs the cavity resonances, changing both their position and linewidth, most noticeably for high quality modes (i.e narrow-line) resonances. This effect is the basis for resonant optical biosensing [1-3]. The changes in the spectral properties of resonators in the presence of perturbations can be used to characterise the size and shape of the attached nanoparticles [4, 5]. The WGM resonances in the microdisks and spherical microcavities have already been used in the characterisation of nanolayers [6], DNA [7] and nano particle detection [8, 9]. Recently, optical resonances have become the core element of a more accurate modeling of multimode and random lasers [10, 11] and of light propagation through random media [12]. In nanoplasmonics, the resonances of metal nanoparticles are used to locally enhance the electromagnetic field [13].

The RSE can also be applied to optical waveguides, which we also studied in this thesis. Optical waveguides are a basic building block for optical technology owing to their low loss guiding of light. Planar WGs with one-dimensional confinement, such as the dielectric slab, and fibre WGs with two-dimensional confinement, are widely used in fibre optic cables for telecommunications, photonic crystal fibres [14], integrated optical circuits [15], and terabit chip to chip interconnects [16].

There already exists numerical techniques for finding eigenmodes such as finite element method (FEM) [17] and the finite difference in time domain (FDTD) method [18] to calculate resonances in open cavities. However determining the effect of perturbations which break the symmetry presents a significant challenge as these popular computational techniques need large computational resources [19] to model high quality modes.

Much of this thesis is taken up with numerical simulations with which we have established the value of the RSE. We have used these numerical results to make comparisons of the RSE performance with available commercial electromagnetic solvers based on FEM or FDTD. Our findings are that the RSE is a few orders of magnitudes more computationally efficient. It therefore has the potential to supersede these presently used methods. To improve the efficiency of the RSE we introduced a local perturbation method for RSE, which is a unique capability of the RSE compared to FEM or FDTD, and allows to calculate small perturbations of a system with a small computational effort. This is especially relevant for sensing or optimization applications. The local perturbation method is an algorithm for selecting modes for inclusion in the basis which make the biggest contribution to the perturbed states of interested, in order to minimise the basis size and computational work load of the RSE.

1.1 RESONANT STATES (RSs) AND THEIR NORMALISA-TION

The concept of resonant states (RSs) was first used by Gamow in 1928 in order to describe the process of radioactive decay, specifically the escape from the nuclear potential of an alpha-particle by tunnelling [20]. Mathematically this corresponded to solving Schrödinger's equation for outgoing boundary conditions (BCs). These states have complex frequency ω with a negative imaginary part meaning their time dependence $\exp(-i\omega t)$ decays exponentially, thus giving an explanation for the exponential decay law of nuclear physics. The further from the decaying system at a given instant of time the greater the wave amplitude, this is a consequence of the exponential decay. An intuitive way of understanding this divergence of wave amplitude with distance is to notice that waves that are further away have left the system at an earlier time when less of the particle probability density had leaked out. Therefore the integral square modulus of the field over all space is infinite, making normalisation a non-trivial task.

RSs are a key concept in the understanding of the GF. Furthermore, in order to use the unperturbed GF expressed as a spectrum of RSs to expand the perturbed RSs in the basis of unperturbed RSs they must be properly normalised.

Our understanding of RSs was greatly improved when we made the observation that the solution to Maxwell's, Schrödinger's, and Dirac's equation are all a source convoluted with their corresponding GF. This immediately allowed us to see RSs and their analytic continuations in the proper place with regard to GF theory. We observed that the analytic continuation of a RS is a solution constructed by convolution between a GF and a source whose frequency tends to that of a pole of the GF with outgoing BCs, where the source amplitude tends to zero in such a way as to exactly compensate the divergence of the GF at that pole. It is clear that in the limit of the source becoming zero the analytic continuation becomes the RS. These observations were our starting point for the derivation we developed of the general 3D normalisation formula for RSs appearing in the spectral GF (see Sec. 2.1 for derivation). The general normalisation formula was first proposed by Muljarov et al in Ref.[21] where a proof for GF equations which are reducible to a scalar form was also included.

In the case of effectively 1D radially symmetric quantum systems described by Schrödinger's equation with only s-wave excitation i.e. the spherically symmetric case excited by a δ source, such as

$$\left[\frac{\partial^2}{\partial r^2} + [k^2 - V(r)]\right] G(r, r') = \frac{2m}{\hbar^2} \delta(r - r'), \qquad (1.1)$$

it was rigorously proven in Ref.[22] that the GF G(r, r') can be written as

$$G(r, r') = \frac{2m}{\hbar^2} \sum_{n} \frac{u_n(r)u_n(r')}{2k_n(k - k_n)},$$
(1.2)

with the normalisation

$$1 = \int_0^a u_n^2 dr + i \frac{u_n^2(a)}{2k_n} \tag{1.3}$$

where the $u_n(r)$ are the RSs of Eq. (1.1) without a source. The surface term in Eq. (1.3) compensates the divergence of the volume integral due to the exponential growth of the RSs with large r. The surface term exponentially increases with a to cancel the exponential increase of the volume integral with increasing a, thus keeping the sum of the terms on the right hand side Eq. (1.3) constant. This was proven by Zel'dovich [23] after considering the integral

$$\lim_{\alpha \to 0} \int_0^\infty u_n(r) e^{-\alpha/r^2} dr \tag{1.4}$$

and the asymptotics of $u_n(r)$ as $r \to \infty$.

At the start of my PhD the tensorial equivalent of Eq. (1.2) for 3D systems not reducible to a scalar equation was lacking derivation. For this thesis we have derived the tensorial equivalent of Eq. (1.2). That derivation began with our idea to investigate convolution of the GF equations and its corresponding Mittag-Leffler GF with a finite oscillating current having a frequency tending to a GF pole. The details of this derivation are given in Appendix B.

The lack of a 3D GF for arbitrary resonators in term of RSs at the start of my PhD was caused by the derivations of such spectral GFs coming from the poles and residues of the analytic GF. The effect of these limitations on the RSE method was that at that time it was only a rigorously proven method for systems reducible to a scalar equation. For systems that can be reduced to a scalar GF equation such as Eq. (1.1) the analytic GF is given by,

$$\mathbf{G}(r,r') = \frac{\phi_L(r_<)\phi_R(r_>)}{W} \tag{1.5}$$

where $\phi_L(r_{<})$ and $\phi_R(r_{>})$ are the left and right solutions of Eq. (1.1) without the delta inhomogeneity. The left (right) solution of the homogeneous equation satisfy the boundary conditions for $r \to 0$ ($r \to \infty$). The Wronskian $W = \phi_L(r)\phi'_R(r) - \phi_R(r)\phi'_L(r)$ in the denominator takes care of the delta inhomogeneity Eq. (1.1). To prove Eq. (1.5) simply substitute it in Eq. (1.1) and integrate over the homogeneity to show it satisfies the GF equation. No equivalent of Eq. (1.5) was known for systems which cannot be reduced to a scalar GF. In fact it is not even always possible in 1D to derive the left and right solutions in Eq. (1.5) analytically, this was the motivation for other authors to develop perturbation methods for effectively 1D systems, we will give details of these theories in the next section.

Another analytic approach to finding the GF of open spherically symmetric 3D systems is found in [24]. The approach is to expand the δ inhomogeneity in Eq. (1.1) into spherical harmonics and the GF into eigenstates of different polarisations and angular momenta. It is then possible to make use of the orthogonality of these eigenstates at real frequencies in order to calculate the expansion coefficients occurring in this GF. Unfortunately this GF is only valid at real frequency as the orthogonality required is the square modulus of the field integrated over all space without surface terms, so is not applicable for the normalisation of complex frequency poles.

A numerical normalisation of RSs for arbitrary three dimensional electrodynamic systems is available in [25]. The approach is to use a perfectly matched layer to absorb the exponentially growing tails of the RSs and thus make numerical volume integrals finite. However we show in this thesis that numerical methods such as FDTD and FEM can be several orders of magnitude less efficient than the RSE for the examples considered (see Sec. 5.2.3).

One approximate solution to the problem of normalising the modes in the spectral representation of the GF for non-symmetric resonators has been to approximate the high quality modes as having real wave vectors outside the resonator [26]. The consequence of this approximation is that the integral of the square modulus of the field is finite, allowing a normalisation by taking just a volume integral of the resonant mode's field inside the resonator only. Such infinitely high quality modes are suitable for lasing modes in lasers and are referred to as constant flux states because the total flux coming from any surface surrounding the laser at lasing threshold is constant. Such an approach is possible since the quality factor for a mode at lasing threshold is infinite. The concept of constant flux states has been used in [27, 28]. For general RSs which have a large range of imaginary parts of their wavevector this approach is not suited.

The normalization constants we find in Sec. 5.1 for a homogeneous sphere are equal to those in Ref.[29] (Eqs. 3.31-3.33), where they are claimed to be resulting from a general formula for the normalization of modes in spherically symmetric systems, Eq. (3.12). However, this formula is different from our normalisation formula, and we found that it diverges for the TE and TM modes, showing that it is incorrect and does not result in Eqs. (3.31-3.33).

1.2 Development of the resonant-state expansion (RSE)

In Ref.[30] More exploited the Dyson equation to express perturbed eigenfunctions of the quantum-mechanical Eq. (1.1) which we label $\hat{u}_n(r)$ with a potential modified by a radially symmetric perturbation $\Delta V(r)$ as

$$\hat{u}_n(r) = \sum_m \frac{u_m(r)}{2k_m(\hat{k}_m - k_m)} \int_0^\infty u_m(r) \Delta V(r) \hat{u}_n(r) dr$$
(1.6)

with perturbed eigenvalues are \hat{k}_m . The summations over perturbed resonant states in the perturbed spectral Green's functions was eliminated by letting $k \to \hat{k}_m$ and comparing residues in the Dyson equation.

In Ref.[31] the completeness of the resonant states allows to write

$$\hat{u}_n(r) = \sum_m c_m u_m(r) \tag{1.7}$$

was used to turn Eq. (1.6) into a linear eigenvalue problem,

$$c_m(\hat{k}_m - k_m) = \sum_n c_n \int_0^\infty \frac{u_m(r)\Delta V(r)u_n(r)}{2k_m} dr.$$
 (1.8)

Prior to my PhD the similarities between Schrödinger's equation and Maxwell's wave equation had already been used to translate the quantum mechanical results we have just touched upon into a similar method for electrodynamics [21]. This perturbation method for electrodynamic RSs is now referred to as the resonant-state expansion (RSE). I note here that applying Eq. (1.8) directly to electrodynamics does not lead to a linear eigenvalue problem.

1.3 Plan of this thesis

In the next chapter we detail our original mathematical derivation of the RSE for arbitrary finite 3D systems. We derive first the spectral representation of the dyadic tensor GF in terms of RSs. We then use this result to derive the normalisation of the RSs. With the spectral GF we are able to formulate the matrix equations for finite systems that can be solved to expand the perturbed RSs in terms of the unperturbed basis which is well know from scalar theories. The RSE for systems invariant in one direction is also developed. Chapter 2 ends with a section detailing the algorithm for error estimation and reduction by extrapolation which we use throughout this thesis to analyse the numerical RSE results.

With this derived method we are able in Chapter 3 to validate the RSE in effectively 1D planar systems with and without an in-plane component of the wave vector. This validation is made possible by the availability of analytic solutions in 1D which we use to calculate the convergence of the RSE to the exact solutions. The role of RSs in the transmission of a dielectric slab is also studied, and in particular the WG modes on the slab transmission.

As a next step towards a 3D implementation of the RSE we apply the method to 2D systems with translational invariance in one direction in Chapter 4. The basis system used is a homogeneous dielectric cylinder. An interesting feature which we found is the presence of a cut in the GF along the imaginary frequency axis. For the accuracy of the RSE the cut must be included in the basis and this is done using a method of discretising the cut into a finite number of poles. We verify this method of discretising the cut for homogeneous perturbations by comparison with analytic solutions and we find that if half the basis is given over to the cut then the error is not significantly limited by the cut. Inclusion of the zero frequency poles were also found to be necessary for the accuracy of the RSE method.

We complete the research component of the thesis with the penultimate chapter where we apply the RSE to 3D systems. The application of the RSE to fully 3D systems opens its use to a very important class of problems. This advance was non-trivial due to a general mixing of transversal and longitudinal electro-magnetic modes. We compare the performance of RSE with available commercial electromagnetic solvers based on FEM or FDTD method, and find that the RSE is a few orders of magnitudes more computationally efficient. It therefore has the potential to supersede these presently used methods. We develop the local perturbation method for the RSE, which is a unique capability of the RSE compared to FEM or FDTD, and allows to calculate small perturbations of a system with a small computational effort. This is especially relevant for optimisation of resonant bio-sensors.

Chapter 2

Formulation of the RSE

In this chapter we will derive the spectral representation of the electrodynamic tensor GF in terms of RSs. We will then consider such a representation of the GF for an unperturbed system and use it to write a matrix equation for the eigenfunctions and eigenfrequencies of a system differing from the unperturbed system by a perturbation to its dielectric profile. We will formulate the RSE both for finite open optical resonators and planar waveguides.

The basis of unperturbed RSs is countably infinite, therefore for the numerical calculations it must be truncated. As the size of the basis is increased the perturbed RSs generated by the RSE converge to the exact solution. At the end of this chapter we develop an algorithm for error estimation and reduction by extrapolation.

2.1 NORMALISATION OF RSS AND THE SPECTRAL REP-RESENTATION OF THE GREEN'S FUNCTION (GF)

We will in this section derive a new method for calculating the GF of an open electrodynamic system. This method is required to formulate the RSE with mathematical rigour.

For an electrodynamic system with local dielectric permittivity tensor $\hat{\boldsymbol{\varepsilon}}(\mathbf{r})$ and permeability $\mu = 1$, where \mathbf{r} is the three-dimensional spatial position, Maxwell's wave equation for the electric field $\mathbf{E}(\mathbf{r})$ with an oscillating current source $\mathbf{J}(\mathbf{r})$ is

$$-\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) + k^2 \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}(\mathbf{r}) = ik \frac{4\pi}{c} \mathbf{J}(\mathbf{r}) \,. \tag{2.1}$$

The time-dependent part of the field is given by $\exp(-i\omega t)$ with the complex eigenfrequency $\omega = ck$, where c is the speed of light in vacuum.

The Green's function (GF) of an open electromagnetic system is a tensor $\hat{\mathbf{G}}_k$ which satisfies Maxwell's wave equation Eq. (2.1) with a δ function source term,

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}'), \qquad (2.2)$$

where $\hat{\mathbf{1}}$ is the unit tensor. Later we use the GF to formulate a matrix equation for the RSs of a perturbed system. In order for the perturbed RSs generated to have outgoing BCs we must use a GF with the same BCs. Physically, the GF describes the response of the system to a point current with frequency $\omega = ck$, i.e. an oscillating dipole.

The importance of $\hat{\mathbf{G}}_k$ comes from the fact we can see from Eq. (2.2) that Eqs. (2.1) can be solved for $\mathbf{E}(\mathbf{r})$ by convolution of $\hat{\mathbf{G}}_k$ with the current source $\mathbf{J}(\mathbf{r})$,

$$\mathbf{E}(\mathbf{r}) = ik\frac{4\pi}{c} \int \hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}') \mathbf{J}(\mathbf{r}) d\mathbf{r}'.$$
(2.3)

Assuming a simple-pole structure of the GF with poles at $k = k_n$ and out going BCs, and taking into account its large-k vanishing asymptotics, the Mittag-Leffler theorem [30, 32] allows us to derive the following expression for the GF

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\hat{\mathbf{Q}}_{n}(\mathbf{r},\mathbf{r}')}{k-k_{n}}.$$
(2.4)

as detailed in Appendix A. In Appendix B we show that

$$\hat{\mathbf{Q}}_{n}(\mathbf{r},\mathbf{r}') = \mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')/2k_{n}, \qquad (2.5)$$

in which the vectorial nature of the field and the symmetry of the kernel Eq. (B.12)

were taken into account and a normalisation constant $2k_n$ was introduced. The direct vector product \otimes is defined as $\mathbf{c}(\mathbf{a} \otimes \mathbf{b})\mathbf{d} = (\mathbf{c} \cdot \mathbf{a})(\mathbf{b} \cdot \mathbf{d})$, for any vectors \mathbf{a} , \mathbf{b} , \mathbf{c} , and \mathbf{d} .

The functions $\mathbf{E}_n(\mathbf{r})$ are the resonant state eigensolutions of the Maxwell wave equation

$$\nabla \times \nabla \times \mathbf{E}_n(\mathbf{r}) = k_n^2 \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_n(\mathbf{r}) , \qquad (2.6)$$

which satisfy the outgoing wave boundary condition, the $r = |\mathbf{r}|$ dependence is given by

$$\mathbf{E}_n(\mathbf{r}) \to r^{-(D-1)/2} e^{ik_n r} \quad \text{for} \ r \to \infty \,, \tag{2.7}$$

where D is the space dimensionality. RSs are either stationary or time-decaying solutions of Maxwell's equation. The wave numbers k_n of time-decaying RSs lie in the lower half of the complex k-plane and come in pairs, having opposite real and equal imaginary parts. Indeed, if $\mathbf{E}_n(\mathbf{r})$ and k_n corresponding to RS n satisfy Eqs. (2.6) and (2.7), taking the complex conjugate of Eq. (2.6) we find that $\mathbf{E}(\mathbf{r}) = \mathbf{E}_n^*(\mathbf{r})$ and $k = \pm k_n^*$ also satisfy the same equation. Only $-k_n^*$ has a negative imaginary part as required for time-decaying solutions since the time dependence is given by the factor $\exp(-ick_n t)$. Here we label the resulting RS with index -n, so that $k_{-n} = -k_n^*$.

Combining Eq. (2.4) and Eq. (2.5) we find

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')}{2k_{n}(k-k_{n})}.$$
(2.8)

Substituting Eq. (2.8) in Eq. (2.2) gives

$$\hat{\boldsymbol{\varepsilon}}(\mathbf{r})\sum_{n}\frac{(k+k_{n})\mathbf{E}_{n}(\mathbf{r})\otimes\mathbf{E}_{n}(\mathbf{r}')}{2k_{n}}=\hat{\mathbf{1}}\delta(\mathbf{r}-\mathbf{r}').$$
(2.9)

Convoluting Eq. (2.9) with a finite field $\mathbf{D}(\mathbf{r})$ which is only non-zero inside the resonator, gives

$$\int_{\Omega} \left(\hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \sum_{n} \frac{(k+k_n) \mathbf{E}_n(\mathbf{r}) \otimes \mathbf{E}_n(\mathbf{r}')}{2k_n} \right) \mathbf{D}(\mathbf{r}') d\mathbf{r}' = \mathbf{D}(\mathbf{r}).$$
(2.10)

Letting $k \to \infty$ in Eq. (2.10) we see that

$$\int_{\Omega} \left(\sum_{n} \frac{\mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')}{2k_{n}} \right) \mathbf{D}(\mathbf{r}') \mathbf{dr}' = \mathbf{0}.$$
 (2.11)

Since Eq. (2.11) is true for all $\mathbf{D}(\mathbf{r})$ it follows that,

$$\sum_{n} \frac{\mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')}{2k_{n}} = 0.$$
(2.12)

Combining Eq. (2.8) and Eq. (2.12) yields

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')}{2k(k-k_{n})}.$$
(2.13)

Combining Eq. (2.9) and Eq. (2.12) leads to the closure relation

$$\frac{\hat{\boldsymbol{\varepsilon}}(\mathbf{r})}{2} \sum_{n} \mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}') = \hat{\mathbf{1}}\delta(\mathbf{r} - \mathbf{r}'), \qquad (2.14)$$

which expresses the completeness of the RSs, so that any function can be written as a superposition of RSs.

For any open system, the RSs form an orthonormal complete set of eigenmodes. It follows from Eq. (2.7) that solutions decaying in time grow exponentially in space as $r \to \infty$. When we derive the orthonormality relation this divergence of the volume integral as $r \to \infty$ is dealt with by involving the electromagnetic energy flux through a surface surrounding the system.

Following Ref.[21] we multiply Eqs. (2.6) by \mathbf{E}_m , repeating the process with mand n exchanged, subtracting the two expressions and integrating the dot product by parts over an arbitrary volume V which includes all system inhomogeneities of $\varepsilon(\mathbf{r})$ the orthogonality of RSs for $n \neq m$ has the form

$$0 = (k_n^2 - k_m^2) \int_V d\mathbf{r} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_n(\mathbf{r}) \cdot \mathbf{E}_m(\mathbf{r}) - \int_{S_V} dS \left(\mathbf{E}_n \cdot \frac{\partial \mathbf{E}_m}{\partial s} - \mathbf{E}_m \cdot \frac{\partial \mathbf{E}_n}{\partial s} \right) , \quad (2.15)$$

where the second integral is taken over the surface S_V surrounding the volume V and contains the gradients $\partial/\partial s$ normal to this surface.

The eigenstates with outgoing boundary conditions must be normalised be used as a basis of the perturbation theory. To this end we consider an analytic continuation $\mathbf{E}(k, \mathbf{r})$ of the wave function $\mathbf{E}_n(\mathbf{r})$ around the point $k = k_n$ in the complex k-plane (k_n is the wavenumber of the given RS). We choose the analytic continuation such that it satisfies the outgoing wave boundary condition and the Maxwell wave equation

$$-\nabla \times \nabla \times \mathbf{E}(k,\mathbf{r}) + k^2 \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}(k,\mathbf{r}) = (k^2 - k_n^2) \boldsymbol{\sigma}(\mathbf{r})$$
(2.16)

with an arbitrary source term corresponding to the current density $\mathbf{j}(\mathbf{r}, k) = \boldsymbol{\sigma}(\mathbf{r})ic(k^2 - k_n^2)/(4\pi k)$. The source $\boldsymbol{\sigma}(\mathbf{r})$ has to be zero outside the volume of the inhomogeneity of $\hat{\boldsymbol{\varepsilon}}(\mathbf{r})$ for the electric field $\mathbf{E}(k, \mathbf{r})$ to satisfy the outgoing wave boundary condition. It also has to be non-zero somewhere inside that volume, as otherwise $\mathbf{E}(k, \mathbf{r})$ would be identical to $\mathbf{E}_n(\mathbf{r})$. We further require that $\boldsymbol{\sigma}(\mathbf{r})$ is normalized according to

$$\int_{V} \mathbf{E}_{n}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r}) \, d\mathbf{r} = 1 + \delta_{k_{n},0} \,, \qquad (2.17)$$

with the Kronecker delta $\delta_{k_n,0} = 1$ for $k_n = 0$ and $\delta_{k_n,0} = 0$ for $k_n \neq 0$. The integral in Eq. (2.17) is taken over an arbitrary simply connected volume V which includes all system inhomogeneities of $\hat{\boldsymbol{\varepsilon}}(\mathbf{r})$. The Eq. (2.17) ensures that the analytic continuation reproduces $\mathbf{E}_n(\mathbf{r})$ in the limit $k \to k_n$. Indeed, solving Eq. (2.16) with the help of the GF and using the GF spectral representation Eq. (2.32), we find

$$\mathbf{E}(k,\mathbf{r}) = \int_{V} \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}')(k^{2}-k_{n}^{2})\boldsymbol{\sigma}(\mathbf{r}')d\mathbf{r}' \qquad (2.18)$$
$$= \sum_{m} \mathbf{E}_{m}(\mathbf{r})\frac{k^{2}-k_{n}^{2}}{2k(k-k_{m})}\int_{V'} \mathbf{E}_{m}(\mathbf{r}') \cdot \boldsymbol{\sigma}(\mathbf{r}') d\mathbf{r}',$$

where we have introduced the sub-volume of V, the volume V' in which $\sigma(\mathbf{r}) \neq 0$. Using Eq. (2.16), Eq. (2.17), Eq. (2.18) and Maxwell's boundary conditions we obtain that for all \mathbf{r}

$$\lim_{k \to k_n} \mathbf{E}(k, \mathbf{r}) = \mathbf{E}_n(\mathbf{r}) \,.$$

In the case of a Green's function made up of degenerate modes the derivation of the normalisation of mode n is modified by making use of orthogonality of the degenerate modes to choose $\sigma(\mathbf{r})$ to satisfy Eq. (2.17) and,

$$\int_{V} \mathbf{E}_{m}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r}) \, d\mathbf{r} = 0 \,, \qquad (2.19)$$

for $m \neq n$ and mode m is degenerate with n.

We now consider the integral

$$I_n(k) = \frac{\int_V (\mathbf{E} \cdot \nabla \times \nabla \times \mathbf{E}_n - \mathbf{E}_n \cdot \nabla \times \nabla \times \mathbf{E}) d\mathbf{r}}{k^2 - k_n^2}$$
(2.20)

and evaluate it using Eqs. (2.6) and (2.16) for \mathbf{E}_n and \mathbf{E} , respectively, and the source term normalization Eq. (2.17)

$$I_n(k) = \frac{\int_V (k_n^2 \mathbf{E} \cdot \hat{\boldsymbol{\varepsilon}} \mathbf{E}_n - k^2 \mathbf{E}_n \cdot \hat{\boldsymbol{\varepsilon}} \mathbf{E}) d\mathbf{r}}{k^2 - k_n^2} + 1 + \delta_{k_n,0}.$$
(2.21)

On the other hand, rearranging the integrand in Eq. (2.20) and using the divergence theorem, we obtain

$$(k^{2} - k_{n}^{2})I_{n}(k) = \oint_{S_{V}} dS \left(\mathbf{E}_{n} \cdot \frac{\partial \mathbf{E}}{\partial s} - \mathbf{E} \cdot \frac{\partial \mathbf{E}_{n}}{\partial s} \right)$$
(2.22)

with S_V being the boundary of V. Here, we used that for two arbitrary vector fields, $\mathbf{a}(\mathbf{r})$ and $\mathbf{b}(\mathbf{r})$, we can write

$$\mathbf{a} \cdot \nabla \times \nabla \times \mathbf{b} - \mathbf{b} \cdot \nabla \times \nabla \times \mathbf{a} =$$
$$\mathbf{a} \cdot [\nabla(\nabla \cdot \mathbf{b}) - \nabla^2 \mathbf{b}] - \mathbf{b} \cdot [\nabla(\nabla \cdot \mathbf{a}) - \nabla^2 \mathbf{a}] =$$
$$\nabla \cdot [\mathbf{a}(\nabla \cdot \mathbf{b}) - \mathbf{b}(\nabla \cdot \mathbf{a})] + \sum_{j=x,y,z} \nabla \cdot (-a_j \nabla b_j + b_j \nabla a_j) .$$

The divergence theorem therefore allows us to convert all volume integrals in Eq. (2.20) into surface integrals over the closed surface S_V , the boundary of V. The surface S_V lies in the region where $\hat{\boldsymbol{\varepsilon}}(\mathbf{r})$ is homogeneous, so that both $\nabla \cdot \mathbf{E}$ and $\nabla \cdot \mathbf{E}_n$ vanish on that surface leaving only the integral shown in Eq. (2.22). Finally, using Eq. (2.21) in Eq. (2.22) and taking the limit $k \to k_n$ we obtain the normalization condition

$$1 + \delta_{k_n,0} = \int_V d\mathbf{r} \mathbf{E}_n(\mathbf{r}) \cdot \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_n(\mathbf{r}) + \lim_{k \to k_n} \frac{\oint_{S_V} dS \left(\mathbf{E}_n \cdot \frac{\partial \mathbf{E}}{\partial s} - \mathbf{E} \cdot \frac{\partial \mathbf{E}_n}{\partial s} \right)}{k^2 - k_n^2}, \quad (2.23)$$

The limit in Eq. (2.23) can be taken explicitly for any spherical surface as found by Muljarov et al in Ref.[21]. In fact, outside the system, where $\hat{\boldsymbol{\varepsilon}}(\mathbf{r}) = \hat{\mathbf{1}}$ (or an isotropic constant) the wave function of any $k_n \neq 0$ mode is given by $\mathbf{E}_n(\mathbf{r}) = \mathbf{F}_n(k_n \mathbf{r})$, where $\mathbf{F}_n(\mathbf{q})$ is a vector function satisfying the equation

$$\nabla_{\mathbf{q}} \times \nabla_{\mathbf{q}} \times \mathbf{F}_n(\mathbf{q}) = \mathbf{F}_n(\mathbf{q}) \tag{2.24}$$

and the Maxwell boundary conditions at system interfaces and at $\mathbf{q} \to \infty$. The analytic continuation of $\mathbf{E}_n(\mathbf{r})$ can be therefore taken in the form

$$\mathbf{E}(k,\mathbf{r}) = \mathbf{F}_n(k\mathbf{r}) \,. \tag{2.25}$$

As in Ref.[21] we may use a Taylor expansion at $k = k_n$ to obtain

$$\mathbf{E}(k,\mathbf{r}) \approx \mathbf{F}_{n}(k_{n}\mathbf{r}) + (k-k_{n})r \left.\frac{\partial \mathbf{F}_{n}(k\mathbf{r})}{\partial(kr)}\right|_{k=k_{n}}$$
$$= \mathbf{E}_{n}(\mathbf{r}) + \frac{k-k_{n}}{k_{n}}r \left.\frac{\partial \mathbf{E}_{n}(\mathbf{r})}{\partial r}\right|$$
(2.26)

and

$$\frac{\partial \mathbf{E}(k,\mathbf{r})}{\partial r} \approx \frac{\partial \mathbf{E}_n(\mathbf{r})}{\partial r} + \frac{k - k_n}{k_n} \frac{\partial}{\partial r} r \frac{\partial \mathbf{E}_n(\mathbf{r})}{\partial r}, \qquad (2.27)$$

where $r = |\mathbf{r}|$ is the radius in the spherical coordinates. Choosing the origin to coincide with the center of the sphere of integration $S_V = S_R$ we note that $\partial/\partial s = \partial/\partial r$ in Eq. (2.23). Substituting Eqs. (2.26) and (2.27) into Eq. (2.23) and taking the limit $k \to k_n$ explicitly leads for $k_n \neq 0$ modes to

$$1 = \int_{V_R} d\mathbf{r} \mathbf{E}_n \cdot \hat{\boldsymbol{\varepsilon}} \mathbf{E}_n + \frac{1}{2k_n^2} \oint_{S_R} dS \left[\mathbf{E}_n \cdot \frac{\partial}{\partial r} r \frac{\partial \mathbf{E}_n}{\partial r} - r \left(\frac{\partial \mathbf{E}_n}{\partial r} \right)^2 \right]$$
(2.28)

where $r = |\mathbf{r}|$, with the origin at the center of the chosen sphere. Static $k_n = 0$ modes, if they exist in the GF spectrum, are normalized according to

$$2 = \int d\mathbf{r} \mathbf{E}_n \cdot \hat{\boldsymbol{\varepsilon}} \mathbf{E}_n \,. \tag{2.29}$$

Their wave functions decay at large distances as $1/r^2$ or quicker, and the volume of integration in Eq. (2.23) can be extended to the full space for which the surface integral is vanishing.

2.2 Formulation of the RSE for finite structures

In this section we consider an unperturbed electrodynamic system for which the RSs are analytically known, and use properties of the GF to make the derivation of the matrix equations for the unknown RSs of a perturbed system written in terms of the RSs of the unperturbed system, this method is the RSE [21]. To make our formulation of the RSE mathematically rigorous we make use of the spectral GF derived in the last section.

The completeness of RSs allows to treat exactly a modified (perturbed) problem

$$\nabla \times \nabla \times \boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = \varkappa_{\nu}^{2} \big[\hat{\boldsymbol{\varepsilon}}(\mathbf{r}) + \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \big] \boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) , \qquad (2.30)$$

in which the RS wave vector \varkappa_{ν} and the electric field \mathcal{E}_{ν} are modified as compared to k_n and \mathbf{E}_n , respectively, due to a perturbation $\Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r})$ with compact support. This problem is treated by (i) solving Eq. (2.30) with the help of the GF,

$$\boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = -\boldsymbol{\varkappa}_{\nu}^{2} \int d\mathbf{r}' \hat{\mathbf{G}}_{\boldsymbol{\varkappa}_{\nu}}(\mathbf{r}, \mathbf{r}') \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}') \boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}'), \qquad (2.31)$$

(ii) using in Eq. (2.31) the spectral representation Eq. (2.13),

$$\boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = -\boldsymbol{\varkappa}_{\nu}^{2} \sum_{n} \mathbf{E}_{n}(\mathbf{r}) \frac{\int d\mathbf{r}' \mathbf{E}_{n}(\mathbf{r}') \cdot \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}') \boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}')}{2\boldsymbol{\varkappa}_{\nu}(\boldsymbol{\varkappa}_{\nu} - k_{n})}, \qquad (2.32)$$

and (iii) expanding the perturbed wave functions into the unperturbed ones,

$$\boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = \sum_{n} b_{n\nu} \mathbf{E}_{n}(\mathbf{r}) \tag{2.33}$$

This is the *RSE method*. The use of the of the unperturbed GF with outgoing BCs is an essential element of the RSE as Eq. (2.31) guarantees that the perturbed wave functions satisfy the same outgoing BCs. The result of using Eq. (2.33) in Eq. (2.32), and equating coefficients of the same basis functions, we obtain a linear matrix eigenvalue problem

$$\varkappa_{\nu} \sum_{m} (\delta_{nm} + V_{nm}/2) b_{m\nu} = k_n b_{n\nu} , \qquad (2.34)$$

which is reduced, using the substitution $b_{n\nu} = c_{n\nu} \sqrt{\varkappa_{\nu}/k_n}$, to the matrix equation

$$\left(\sum_{n} \frac{\delta_{nm}}{k_m} + \frac{V_{nm}}{2\sqrt{k_n k_m}}\right) c_{m\nu} = \frac{1}{\varkappa_{\nu}} c_{n\nu} \,. \tag{2.35}$$

This allows us to find the wave vectors \varkappa_{ν} and the expansion coefficients $c_{n\nu}$ of the perturbed RSs by diagonalizing a complex symmetric matrix. The matrix elements of the perturbation are given by

$$V_{nm} = \int \mathbf{E}_n(\mathbf{r}) \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_m(\mathbf{r}) \, d\mathbf{r} \,. \tag{2.36}$$

In spite of the exponentially growing \mathbf{E}_n outside the system, the perturbation $\Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \neq 0$ only inside the system so that V_{nm} is always finite.

2.3 Formulation of the RSE for planar wave guides

In the previous section the RSE was applied to finite resonators. When a resonator has translational invariance it is possible for electromagnetic waves to propagate along the directions of this invariance, in which case the system becomes a waveguide. In this section we present the perturbation theory for resonators with translational invariance in two dimensions and non-normal incidence at the interface, characterized by an in-plane wave vector component $p \neq 0$. The previously used spectral representation of the GF in the frequency domain contains a cut for $p \neq 0$, however this can be removed by mapping the problem onto the complex normal wavevector space k. We will discuss this cut in Sec. 3.1, Sec. 3.3, and Sec. 3.4. Therefore the RSE is reformulated in the complex k-plane.

Following the approach of the previous section first the spectral representation of the GF is established, which will then be used to formulate a matrix equation for the perturbed RSs. This matrix problem which can be solved to expand the perturbed RSs in terms of unperturbed RSs is known as the RSE for inclined geometry. Future development of the RSE for inclined geometry will include extending this treatment to systems with one dimension of translational invariance to provide an efficient algorithm for calculating the optical modes in fibers and waveguides, such as photonic crystal fibers with complex structures.

The electric field **E** satisfies Maxwell's equation Eq. (2.1) and Maxwell's boundary conditions on the dielectric/vacuum interfaces. We limit the treatment here to TE modes. For an incoming plane monochromatic wave with the transverse-electric (TE) polarization along \hat{y} (\hat{y} is the unit vector along the *y*-axis) and real frequency ω , the electric field in the system takes the form

$$\mathbf{E}(\mathbf{r},t) = \hat{y}e^{-i\omega t + ipx}E(z), \qquad (2.37)$$

in which p is the in-plane projection of the wave vector, which is taken to be in the x direction without loss of generality. For the component E(z) of the electric field and $\mathbf{J}(\mathbf{r}) = 0$, Eq. (2.1) results in the 1D wave equation

$$\left[\frac{d^2}{dz^2} - p^2 + \varepsilon\left(z\right)\frac{\omega^2}{c^2}\right]E(z) = 0, \qquad (2.38)$$

and the GF satisfies the equation

$$\left[\frac{d^2}{dz^2} - p^2 + \varepsilon(z)(k^2 + p^2)\right] G_k(z, z') = \delta(z - z').$$
(2.39)

The spectral representation of the GF of an infinite planar system with an in-plane momentum $p \neq 0$ has the form

$$G_k(z, z') = \sum_n \frac{E_n(z)E_n(z')}{2k_n(k - k_n)},$$
(2.40)

where $E_n(z)$ is the electric field of the n^{th} RS and k_n the normal projection of its wave vector, defined as an eigensolution of Eq. (2.38) with an arbitrary profile of $\varepsilon(z)$ within a finite interval |z| < a, with a vacuum in the region |z| > a, satisfying the outgoing wave BCs

$$E_n(z) \propto e^{ik_n|z|} \quad \text{for} \quad |z| > a \tag{2.41}$$

and orthonormality conditions derived using the method of Section 2.1, following from Eq. (2.23),

$$\int_{-a}^{a} \varepsilon(z) E_n(z) E_m(z) \, dz - \frac{E_n(-a) E_m(-a) + E_n(a) E_m(a)}{i(k_n + k_m)} = \delta_{nm}.$$
 (2.42)

Following the derivation in the last section we arrive at the sum rule:

$$\sum_{n} \frac{E_n(z)E_n(z')}{k_n} = 0.$$
 (2.43)

For p = 0 the right-hand side of the above sum rule is replaced by i, due to the k = 0pole of the GF which is not present in the spectrum for $p \neq 0$ [21]. Using Eq. (2.43), we can write Eq. (2.40) as

$$G_k(z, z') = \sum_n \frac{E_n(z)E_n(z')}{2k_n} \left[\frac{1}{k - k_n} + F(k)\right], \qquad (2.44)$$

where F(k) is an arbitrary function which will be appropriately chosen later, in order to linearize a resulting matrix eigenvalue problem of the RSE. An arbitrary perturbation $\Delta \varepsilon(z)$ of the dielectric constant inside the resonator is now considered. The perturbed RS with electric field $\mathcal{E}_{\nu}(\mathbf{r})$ and normal component of wave vector \varkappa_{ν} is related to the unperturbed one via

$$\boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = -(\boldsymbol{\varkappa}_{\nu}^{2} + p^{2}) \int d\mathbf{r}' \hat{\mathbf{G}}_{\boldsymbol{\varkappa}_{\nu}}(\mathbf{r}, \mathbf{r}') \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}') \boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}'), \qquad (2.45)$$

Substituting Eq. (2.44) into Eq. (2.45) results in the following relationship between unperturbed and perturbed modes

$$\mathcal{E}_{\nu}(z) = -\left(\varkappa_{\nu}^{2} + p^{2}\right) \sum_{n} \frac{E_{n}(z)}{2k_{n}} \left[\frac{1}{\varkappa_{\nu} - k_{n}} + F(\varkappa_{\nu})\right] \int_{-a}^{a} E_{n}(z') \Delta \varepsilon(z') \mathcal{E}_{\nu}(z') dz'.$$
(2.46)

Note that the perturbed modes $\mathcal{E}_{\nu}(z)$ satisfy Maxwell's equation with $\varepsilon(z)$ replaced by $\varepsilon(z) + \Delta \varepsilon(z)$ and the BCs Eq. (2.41) with normal incidence wavevector component k_n replaced by \varkappa_{ν} . In the interior region |z| < a which contains the perturbation, the perturbed RSs can be expanded into the unperturbed ones, exploiting the completeness of the RSs inside the resonator:

$$\mathcal{E}_{\nu}(z) = \sum_{n} b_{n\nu} E_n(z) \,. \tag{2.47}$$

Substituting this expansion into Eq. (2.46) and equating coefficients at the same basis functions $E_n(z)$ results in the matrix equation

$$b_{n\nu} = -\frac{\varkappa_{\nu}^2 + p^2}{2k_n} \left[\frac{1}{\varkappa_{\nu} - k_n} + F(\varkappa_{\nu}) \right] \sum_m V_{nm} b_{m\nu} , \qquad (2.48)$$

where

$$V_{nm} = \int_{-a}^{a} \Delta \varepsilon(z) E_n(z) E_m(z) dz \qquad (2.49)$$

is the matrix of the perturbation in the basis of unperturbed RSs.

Equation (2.48) is a matrix eigenvalue problem which can be solved numerically in order to find the wave vectors \varkappa_{ν} and the corresponding eigenfrequencies of the perturbed RSs, as well as their expansion coefficients $b_{n\nu}$ in terms of the unperturbed ones. However, this problem is generally nonlinear in \varkappa_{ν} , as can be seen by choosing F(k) = 0. Nonlinear eigenvalue problems are known to take longer to solve and demand more computer memory while at the same time being prone to instabilities and spurious solutions. These problems are avoided by choosing

$$F(k) = -\frac{k}{k^2 + p^2} = -\frac{kc^2}{\omega^2},$$
(2.50)

explicitly depending on the in-plane wave vector p, in order to linearise the eigenvalue problem. Indeed, with the substitution $c_{n\nu} = b_{n\nu}\sqrt{k_n/\varkappa_{\nu}}$, the eigenvalue problem Eq. (2.48) is given by

$$\sum_{m} \left(\frac{\delta_{nm}}{k_n} + \frac{V_{nm}}{2\sqrt{k_n k_m}} \right) c_{m\nu} = \frac{1}{\varkappa_{\nu}} \sum_{m} \left(\delta_{nm} - \frac{p^2 V_{nm}}{2k_n \sqrt{k_n k_m}} \right) c_{m\nu}$$
(2.51)

which is *linear* and can be solved by inverting the matrix on the right-hand side of Eq. (2.51) and diagonalizing the resulting non-symmetric matrix on the left-hand side, in order to obtain its eigenvalues $1/\varkappa_{\nu}$. Alternatively, we can solve Eq. (2.51) by employing a variety of software libraries available for generalized linear matrix eigenvalue problems. Note that the matrix equation of the RSE for normal incidence previously derived in Ref.[21] is restored by choosing p = 0 in Eq. (2.51). The perturbation method in this section will be applied in Chapter 3

2.4 Convergence and extrapolation

It will be shown throughout this work that as the number of basis states N used to calculate a given perturbed RS is increased there is convergence to the exact solution. It was noted earlier [21] that for a uniform perturbation of a wide layer of a 1D slab this convergence was following a N^{-3} scaling. We show in the next chapter that for the 1-dimensional case the convergence is following a power law in the basis size, which allows to estimate the remaining error for finite basis sizes. Furthermore, an extrapolation algorithm is developed which uses this scaling to significantly improve the accuracy of the RS frequencies.

First we assume that the absolute error, i.e the difference between the RS wave

number calculated via the RSE $\varkappa_{\nu}^{(N)}$ and its exact value $\varkappa_{\nu}^{(\text{exact})}$ scales as a power law in the basis size N:

$$\varkappa_{\nu}^{(\text{exact})} - \varkappa_{\nu}^{(N)} \approx K_{\nu} N^{\alpha_{\nu}}.$$
(2.52)

We make a second assumption that the exponent in the power law (α_{ν}) is a real number, so that the RS wave numbers converge in a straight line in the complex plane. The extrapolation is only used if these assumptions are met for a range of N as will be detailed later. The model for the numerical error given by Eq. (2.52) is only used if the power law is being followed by the convergence of the RSs sufficiently well so as for extrapolation by this model to improve the accuracy of the RSs.

To determine K_{ν} , α_{ν} and $\varkappa_{\nu}^{(\text{exact})}$ in Eq. (2.52) from the RSE, $\varkappa_{\nu}^{(N)}$ is needed for a minimum of three different N. In order to estimate the error of the extrapolation, we uses two triplets, namely $\{N_1, N_2, N_4\}$, yielding K'_{ν} , α'_{ν} , and $\{N_2, N_3, N_4\}$, yielding K''_{ν} , α''_{ν} . This allows to calculate K_{ν} , α_{ν} twice for the purposes of estimating the error from the reproducibility of these parameters. We choose the sizes as

$$N_1 \approx \eta^4 N_4, \quad N_2 \approx \eta^2 N_4, \quad N_3 \approx \eta N_4,$$
 (2.53)

with the factor $0 < \eta < 1$, yielding analytic expressions as shown later.

For each basis size the set of RS is calculated with the RSE. The RSs are matched between the four sets sequentially, *i.e.* first $\{\varkappa_{\nu}^{(N_4)}\}$ to $\{\varkappa_{\nu}^{(N_3)}\}$, then $\{\varkappa_{\nu}^{(N_3)}\}$ to $\{\varkappa_{\nu}^{(N_2)}\}$, and finally $\{\varkappa_{\nu}^{(N_2)}\}$ to $\{\varkappa_{\nu}^{(N_1)}\}$. In doing this, the following matching algorithm (MA) is used between the two sets of wave numbers, $\{\varkappa_{\nu}^{(A)}\}$ and $\{\varkappa_{\nu}^{(B)}\}$:

- (a) Determine the distance between the complex wave numbers of all pairs with one element from $\{\varkappa_{\nu}^{(A)}\}$ and one element from $\{\varkappa_{\nu}^{(B)}\}$.
- (b) Select the pair with the shortest distance, store it, and remove all pairs containing one of the elements of the selected pair from the sets.
- (c) Repeat (b) until $\{\varkappa_{\nu}^{(A)}\}$ or $\{\varkappa_{\nu}^{(B)}\}$ is empty.

This procedure results in N_1 vectors $(\varkappa_{\nu}^{(N_1)}, \varkappa_{\nu}^{(N_2)}, \varkappa_{\nu}^{(N_3)}, \varkappa_{\nu}^{(N_4)})$ of RS wave numbers.

The specific factors chosen between N_1 , N_2 , N_3 , and N_4 allow for the following analytical expressions for two sets of coefficients and exponents in Eq. (2.52), for each state ν :

$$\alpha'_{\nu} = \frac{1}{2\ln\eta} \ln\left(\left| \frac{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_1)}}{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_2)}} \right| - 1 \right), \qquad (2.54)$$

$$\alpha_{\nu}'' = \frac{1}{\ln \eta} \ln \left(\left| \frac{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_2)}}{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_3)}} \right| - 1 \right), \qquad (2.55)$$

$$K'_{\nu} = \frac{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_2)}}{N_2^{\alpha'_{\nu}} - N_4^{\alpha'_{\nu}}}, \qquad (2.56)$$

$$K_{\nu}'' = \frac{\varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_3)}}{N_3^{\alpha_{\nu}''} - N_4^{\alpha_{\nu}''}}.$$
(2.57)

For extrapolation of eigenvalues and estimation of errors we use the mean values

$$\alpha_{\nu} = \frac{\alpha_{\nu}' + \alpha_{\nu}''}{2}, \quad K_{\nu} N_4^{\alpha_{\nu}} = \frac{K_{\nu}' N_4^{\alpha_{\nu}'} + K_{\nu}'' N_4^{\alpha_{\nu}''}}{2}.$$
 (2.58)

In order to test the quality of our power law fit, we estimate for each state ν the relative extrapolation error which we define as

$$F_{\nu} = \Phi(K'_{\nu}N_4^{\alpha'_{\nu}}, K''_{\nu}N_4^{\alpha''_{\nu}}), \qquad (2.59)$$

where $2\Phi(X, Y) = \Gamma(X, Y) + \Gamma(Y, X)$ and

$$\Gamma(X,Y) = \left|\frac{X}{Y} - 1\right|.$$
(2.60)

We find from algebra in the complex plane that F_{ν} has the meaning of a relative error in the power law approximation of the distance $\varkappa_{\nu}^{(\text{exact})} - \varkappa_{\nu}^{(N_4)}$ deduced from the two sets of power law parameters. If this error is sufficiently small, $F_{\nu} < F_{\text{max}}$, and the power law converges sufficiently fast ($\alpha_{\nu} < \alpha_{\text{max}}$), we can improve the result calculated for the largest basis size N_4 by extrapolating it towards the exact value, $\varkappa_{\nu}^{(N_4)} \rightarrow \varkappa_{\nu}^{(\infty)}$, where the extrapolated wave vector $\varkappa_{\nu}^{(\infty)}$ is defined according to Eq. (2.52) as

$$\varkappa_{\nu}^{(\infty)} = \varkappa_{\nu}^{(N_4)} + K_{\nu} N_4^{\alpha_{\nu}}.$$
(2.61)

Otherwise, the power law is not describing the convergence well. In that case we then use the absolute variation scaled to the system size

$$M_{\nu} = \max_{i=1,2,3} \left| \varkappa_{\nu}^{(N_4)} - \varkappa_{\nu}^{(N_i)} \right| a , \qquad (2.62)$$

to evaluate if the state has sufficiently converged.

We will use state ν for the calculation of the Greens function and/or transmission if its relative or absolute error is sufficiently small, *i.e.* if one of the two selection criteria (SC) is met:

- 1. extrapolation error $F_{\nu}|K_{\nu}N_{4}^{\alpha_{\nu}}|a < M_{\max}$ provided that $F_{\nu} < F_{\max}$ and $\alpha_{\nu} < \alpha_{\max}$;
- 2. absolute error $M_{\nu} < M_{\max}$.

For the results shown in this thesis we used $M_{\text{max}} = 0.1$, $F_{\text{max}} = 1$, $\alpha_{\text{max}} = -0.5$, and $\eta = 2^{-1/4}$.

We estimate the resulting numerical complexity of this method as follows. For a sufficiently large basis size N, the numerical complexity calculating the RS wave numbers is governed by the time required for diagonalization of an $N \times N$ complex matrix scaling as N^3 . To produce the four sets of RS used above, the complexity is $(1 + \eta^3 + \eta^6 + \eta^{12})N_4^3 \approx 2N_4^3$.

The method of analysing results presented in this section is used for all the numerical results shown in the subsequent chapters.

2.5 SUMMARY

In this chapter we have formulated the RSE for open optical systems. To this end we use a GF for the unperturbed system and the perturbation to formulate a
matrix equation which can be solved to give an expansion of the perturbed RSs in terms of a basis of unperturbed RSs. This was achieved by expressing the spectral GF in terms of normalised resonant states. The key idea that unlocked this theoretical development was the use of a Mittag-Leffler expansion of the GF to analytically express RSs and their corresponding analytic continuations.

In addition to these theoretical developments we have also developed algorithms which can be used to estimate the error in the RS wavenumbers, and to extrapolate them. This is possible because the perturbed RS wavenumbers of the RSE converge to the exact solution as the number of RSs used in the RSE is increased.

Chapter 3

RSE applied to one-dimensional open optical systems

In this chapter, the RSE is applied to calculate RS and transmission/scattering properties of an open optical system, and its performance is investigated on several planar structures for which analytic and numerical solution of high accuracy are available for comparison.

The spectrum of RSs for normal incidence consists only of lossy Fabry-Perot (FP) modes. However for waveguides (WGs) the spectrum includes WG and antiwaveguide (AWG) modes, as well as a continuum of modes due to a cut of the Green's function in the complex frequency plane. The modes on the cut contribute significantly to the optical spectra and are required for the completeness of the RS basis. They present a challenge in the technical implementation of the RSE which is dealing with discrete states. In this chapter, the cut is eliminated in the planar systems with $p \neq 0$ by going from the frequency representation of the system to the normal wave-vector representation.

For the planar system with normal incidence in Sec. 3.2 we investigate the accuracy with which eigenfrequencies, eigenfunctions, the Green's function, and transmission can be reproduced. We apply the RSE to a perturbed dielectric slab in Sec. 3.2 with two different types of perturbations: a wide-layer perturbation, and a δ -perturbation. We find that the RSE converges to the exact solution with a power law in the basis size. As a prelude to later chapters where whispering gallery mode are treated, we treat a Bragg mirror microcavity in Sec. 3.2.5, an example of a structure with a sharp resonance and show that in this case the RSE reproduces results of the scattering matrix method.

For $p \neq 0$ a study is made in Sec. 3.3 of the transmission of a homogeneous slab in the complex frequency and normal wave vector plane, in order to analyse the contributions of different types of RSs to its optical spectra. In Sec. 3.4 we treat different planar structures and compare results with available exact solutions. In particular, we examine in Sec. 3.4.1 the basis of RSs for a homogeneous slab in inclined geometry and then use it for calculation of optical modes of a homogeneous slab with a different refractive index in Sec. 3.4.2 and of a Bragg-mirror microcavity in Sec. 3.4.3.

3.1 EIGENMODES OF A HOMOGENEOUS DIELECTRIC SLAB AS BASIS FOR THE RSE

In this section we will give the eigenmodes of the homogeous 1D planar slab which are used as the basis for the RSE throughout this chapter. We consider electrodynamic systems with both zero and non-zero in-plane momentum.

The unperturbed system can be any convenient system. In the discussed 1D case, a dielectric slab in vacuum having a thickness 2a and a real dielectric constant

$$\varepsilon(z) = \begin{cases} \epsilon_s & \text{for } |z| < a \\ 1 & \text{otherwise} \end{cases}$$
(3.1)

is the simplest 1-dimensional system, and has an analytic solution. In this chapter it is taken as the unperturbed system.

For the transverse-electric (TE) polarisation we use symmetry in 1D to write the solution to Maxwell wave equation for the RSs, Eq. (2.30), as

$$\mathbf{E}_{n}(\mathbf{r}) = \hat{y}e^{-ick_{n}t + ipx}E_{n}(z), \qquad (3.2)$$

since for the component of $E_n(z)$ of the electric field, Eq. (2.30) transforms to a 1D wave equation. The in-plane projection of the wave vector is p and the projection normal to the planar structure is k_n .

$$\left[\frac{d^2}{dz^2} - p^2 + \varepsilon\left(z\right)\frac{\omega^2}{c^2}\right]E(z) = 0.$$
(3.3)

We are dictated by the formalism of the RSE to use outgoing boundary conditions for the RSs.

In 1D the electric field of RS n is normalized according to Eq. (2.23), which in 1D takes the form

$$\int_{-a}^{a} \varepsilon(z) E_n(z) E_m(z) \, dz - \frac{E_n(-a) E_m(-a) + E_n(a) E_m(a)}{i(k_n + k_m)} = \delta_{nm} \,, \qquad (3.4)$$

The solutions for the RSs in Eq. (3.3) with the profile of the dielectric constant $\varepsilon(z)$ given by Eq. (3.1) take the form

$$E_{n}(z) = \begin{cases} (-1)^{n} A_{n} e^{-ik_{n}z}, & z \leqslant -a, \\ B_{n}[e^{iq_{n}z} + (-1)^{n} e^{-iq_{n}z}], & |z| \leqslant a, \\ A_{n} e^{ik_{n}z}, & z \geqslant a, \end{cases}$$
(3.5)

where the normal wave-vector space eigenvalues k_n satisfy the secular equation

$$(k_n - q_n) e^{iq_n a} + (-1)^n (k_n + q_n) e^{-iq_n a} = 0, \qquad (3.6)$$

with $q_n = \sqrt{\epsilon_s k_n^2 + (\epsilon_s - 1)p^2}$. We use here an integer index *n* which takes even (odd) values for symmetric (anti-symmetric) RSs, respectively. The normalization constants A_n and B_n are found from the continuity of E_n , the continuity of the tangential magnetic field across the boundaries, and the normalization condition Eq. (3.4). They

take the form

$$A_n = \frac{e^{-ik_n a}}{\sqrt{a(\epsilon_s - 1)}} \sqrt{\frac{\epsilon_s \omega_n^2 / c^2 - p^2}{\epsilon_s \omega_n^2 / c^2 + ip^2 / (k_n a)}}, \qquad (3.7)$$

$$B_n = \frac{(-i)^n}{2\sqrt{a\epsilon_s + ip^2/(k_n\omega_n^2/c^2)}},$$
(3.8)

where $\omega_n^2/c^2 = k_n^2 + p^2$.

The RS wave vectors in the case of normal incidence p = 0 can be calculated from Eq. (3.6) and are given by

$$k_n = \frac{1}{2a\sqrt{\epsilon_s}}(\pi n - i\ln\gamma), \qquad n = 0, \pm 1, \pm 2, \dots,$$
(3.9)

with

$$\gamma = \frac{\sqrt{\epsilon_s} + 1}{\sqrt{\epsilon_s} - 1},\tag{3.10}$$

all having the same imaginary part.



Figure 3.1: Poles (symbols) and cut (red lines) of the transmission $\tilde{t}(\omega)$ of a homogeneous dielectric slab with $\epsilon_s = 9$ and in-plane wave vector pa = 5. The poles are Fabry-Perot (blue crosses), waveguide (black diamonds) and anti-waveguide modes (open circles) including a leaky mode (open star). The inset shows the absence of $\omega = 0$ and k = 0 modes.

An example of the poles appearing in the complex frequency plane of a planar

electrodynamic system with non-zero in-plane momentum is shown in Fig. 3.1. As in the case of normal incidence, there are a countable infinite number of FP modes having nearly equidistant real parts and finite imaginary parts. In addition there are two types of modes on the real ω -axis: WG and AWG modes, which are appearing for $p \neq 0$. The WG modes have an evanescent, i. e. exponentially decaying electric field into the vacuum, while the AWG modes are exponentially growing into the vacuum and are known in quantum-mechanics as anti-bound states [33]. Finally there is one leaky mode (LM) at the center of the spectrum which has zero real and negative imaginary part of ω . Importantly Fig. 3.1 shows a cut in the transmission in ω space which due to the use of the residue theorem (see Appendix A) would need to appear in the basis of RSs, if one formulated the RSE in ω space. Fortunately this cut does not appear in Eq. (3.6), the transcendental equation in terms of the component of the wave vector projected in the direction normal to the planar system. This explains why the RSE is formulated in terms of the component of the wave vector projected in the direction normal to the planar system.

The number of RS in the unperturbed or perturbed systems is countable infinite. Therefore we always deal with a truncation of the basis of the RS made symmetrically in the complex plane of k, where k is the component of the wave vector normal to the planar system. Hence we choose some k_{max} and select all $|k_n| \leq k_{\text{max}}$. This truncation is the only approximation of the theory. We refer to n_{max} as the truncation number for the basis so that $-n_{\text{max}} \leq n \leq n_{\text{max}}$. For normal incidence p = 0 the basis size N is given by

$$N = 2n_{\max} + 1. (3.11)$$

By choosing the basis size N sufficiently large, the results of the perturbation theory can be produced with any given accuracy.

3.2 Numerical results for normal incidence

In this section we report results of the RSE applied to a planar open electrodynamic system with zero in-plane moment (p = 0). We make use of exact solutions which are available for these simple geometries to verify the accuracy of the numerical calculations required in the RSE so as to justify further development of the method in subsequent chapters of this thesis.

We find the perturbed modes by solving the generalised eigenvalue problem given by Eq. (2.51). The matrix elements V_{nm} are given by

$$V_{nm} = \int_{-a}^{a} \Delta \varepsilon(z) E_n(z) E_m(z) dz , \qquad (3.12)$$

where E_n are given in Eq. (3.5).

3.2.1 WIDE-LAYER PERTURBATION

The perturbation being considered in this subsection is given by

$$\Delta \varepsilon(z) = \begin{cases} \Delta \epsilon & \text{for } a/2 \le z \le a ,\\ 0 & \text{otherwise} \end{cases}$$
(3.13)

with $\Delta \epsilon = 10$. The profiles of the unperturbed and perturbed dielectric constants are shown in Fig. 3.2. The analytic solutions of the time-independent Maxwell's equations using the RS boundary conditions are given in Appendix C, for perturbed systems, along with the matrix elements V_{nm} of the perturbation. Using the procedure introduced in Sec. 2.4 we calculate four sets of perturbed wave numbers and extrapolate \varkappa_{ν} according to Eq. (2.61). We also calculate the exact wave numbers $\varkappa_{\nu}^{(\text{exact})}$ and match up exact and perturbed states using the matching algorithm described in Sec. 2.4. The resulting exact and extrapolated eigenvalues $\varkappa_{\nu}^{(\infty)}$ are shown in the inset of Fig. 3.3, together with the unperturbed wave vectors. We measure the errors in $\varkappa_{\nu}^{(\infty)}$ relative to $\varkappa_{\nu}^{(\text{exact})}$ by $\Gamma(\varkappa_{\nu}^{(\infty)}, \varkappa_{\nu}^{(\text{exact})})$ and compare it with $\Gamma(\varkappa_{\nu}^{(N_4)}, \varkappa_{\nu}^{(\text{exact})})$ to evaluate the extrapolation method, where the Γ function is defined in Sec. 2.4. The results are



Figure 3.2: Dielectric constants of the unperturbed slab $\varepsilon(z)$ and a slab with a wide perturbation $\varepsilon(z) + \Delta \varepsilon(z)$.

shown in Fig. 3.3. We see that the relative error of the RS wave number is generally reduced by extrapolation by more than one order of magnitude.

The coefficients and exponents of the power law fit give us information about the convergence properties of the perturbed RS. For the wide perturbed layer they are shown in Fig. 3.4. We see in Fig. 3.4 (a) that states close to the origin in complex wave number space (and having small state number values) are not described well by the power law (The estimated relative extrapolation error F_{ν} is larger than F_{max}), even though Fig. 3.3 suggests that these states are well converged. This is reflected in the small absolute error M_{ν} shown in Fig. 3.4(g),(h), passing the selection criteria (SC) for extrapolation of Sec. 2.4. We also see that for higher wave-number states passing the SC the exponent in the power law is close to $\alpha = -3$ [horizontal lines in Fig. 3.4 (c),(d)], in accordance with the findings in Ref.[21].

Furthermore, the absolute errors $K_{\nu}N^{\alpha_{\nu}}$ and M_{ν} show universal dependencies on the normalized state number ν/n_{max} , as shown in Fig. 3.4 (f) and (h). This provides us with a scaling law of the absolute errors versus the state number:

$$M_{\nu} \propto (\nu/N)^3 \,. \tag{3.14}$$

This cubic scaling is shown in Fig. 3.4(f), (h) by straight magenta lines. The power



Figure 3.3: Relative errors $\Gamma(\varkappa_{\nu}^{(\infty)}, \varkappa_{\nu}^{(\text{exact})})$ and $\Gamma(\varkappa_{\nu}^{(N_4)}, \varkappa_{\nu}^{(\text{exact})})$ of the RS wave vectors calculated via the RSE for the perturbation shown in Fig. 3.2, with and without extrapolation, respectively, for $N_4 = 801$. Inset: unperturbed and perturbed RS wave numbers; the latter are calculated analytically (empty squares) and via the RSE with extrapolation (crosses).

law exponent α also shows a universal dependency on the normalized state number, being $\alpha = -3$ for $\nu/n_{\text{max}} \lesssim 0.2$ as can be seen in Fig. 3.4 (d). In this region the states pass the relative SC and are extrapolated. An example of how the power law is applied to extrapolate the wave number of a particular state $\nu = 63$ is given in Fig. 3.5 (a). Clearly, the extrapolation leads to a considerable improvement of the accuracy compared to wave numbers calculated with the maximum matrix size N_4 . This is due to the good power law convergence as shown in Figure 3.5 (b), seen by the straight line connecting the "exact" errors $|\varkappa_{\nu}^{(\text{exact})} - \varkappa_{\nu}^{(N_i)}|$ for the four basis sizes. The exact errors are only available if the exact solution is known. In a realistic case for which no such solution is known, one needs to estimate the error of the power law extrapolation, as we do using the extrapolation SC and Eq. (2.59). In order to check how good this estimation is, we compare F_{ν} with the exact relative extrapolation error $F_{\nu}^{(\text{exact})} = \Phi(K_{\nu}N_4^{\alpha_{\nu}}, \varkappa_{\nu}^{(\text{exact})} - \varkappa_{\nu}^{(N_4)})$. Such a comparison is shown in Fig. 3.6



Figure 3.4: Power law parameters and error estimates for the wide perturbation. (a),(b): Relative extrapolation error F_{ν} . (c),(d): exponent α_{ν} in the power law fit. (e),(f): absolute errors $K_{\nu}N^{\alpha_{\nu}}$ and (g),(h): M_{ν} as function of the the state number ν , calculated for different basis size N. The right panels display the data versus the state number ν normalized to its maximum value $n_{\max} = (N-1)/2$. Straight magenta lines are $\alpha = -3$ (c),(d) and power law fits (h),(f).



Figure 3.5: (a) Wave number of the perturbed state $\nu = 63$ calculated with different basis sizes N and extrapolated to the exact value. (b) Absolute "exact" error $|\varkappa_{63}^{(\text{exact})} - \varkappa_{63}^{(N)}|$ for different N (squares) and a power law fit (dashed line).

for all states with $\alpha_{\nu} < -0.5$. We can see that the exact error $F_{\nu}^{(\text{exact})}$ is typically overestimated by F_{ν} , and for all states with $F_{\nu} < F_{\text{max}}$ we have $F_{\nu}^{(\text{exact})} < 1$, i.e. the extrapolation is improving the error. F_{ν} can thus be used reliably to verify the convergency and power law extrapolation.

3.2.2 ELECTRIC FIELDS

The electric fields (EF) $\mathcal{E}_{\nu}(z)$ of the perturbed RS calculated via the exact formula Eq. (C.1) are shown in Fig. 3.7 for a few lowest states in comparison with $E_n(z)$, the EF of the unperturbed RS, given by Eq. (3.5). The perturbed RS are normalized as in Eq. (3.4). In particular, their orthonormality condition reads



Figure 3.6: "Exact" relative extrapolation error $F_{\nu}^{(\text{exact})}$ versus relative extrapolation error F_{ν} for both accepted and rejected states, for $N_4 = 801$. The blue dashed line shows the anticipated behavior $F_{\nu}^{(\text{exact})} \approx F_{\nu}$.

$$\int_{-a}^{a} \varepsilon_{p}(z) \mathcal{E}_{\nu}(z) \mathcal{E}_{\mu}(z) dz - \frac{\mathcal{E}_{\nu}(-a)\mathcal{E}_{\mu}(-a) + \mathcal{E}_{\nu}(a)\mathcal{E}_{\mu}(a)}{i(\varkappa_{\nu} + \varkappa_{\mu})} = \delta_{\nu\mu}, \qquad (3.15)$$

where $\varepsilon_p(z) = \varepsilon(z) + \Delta \varepsilon(z)$ is the perturbed dielectric profile. All unperturbed states have the same imaginary part of their wave vectors (see the inset in Fig. 2) and thus their fields have all the same envelope, exponentially growing outside the slab, with the higher-*n* states oscillating more rapidly, see Fig. 3.7 (a). In the perturbed system, the envelopes are different due the varying Im \varkappa_{ν} . Also, as can be seen in Fig. 3.7(b), the frequency of the oscillations increases in the perturbed (denser) layer, and their amplitudes change at the same time.

The perturbation theory fully reproduces the EF of the RS inside the slab. Inside the slab, the EF is given by the expansion in Eq. (2.33) with the coefficients $c_{n\nu}$ diagonalizing the matrix in Eq. (2.35). To quantify how well the perturbation theory reproduces the EF of a RS, we make use of the root mean square (RMS)



Figure 3.7: Real part of the normalized electric field of a few lowest energy RS of the unperturbed slab (a) and of the perturbed slab (b).

deviation within the system defined by

$$\Delta_{\nu} = \sqrt{\frac{\int_{-a}^{a} \left| \mathcal{E}_{\nu}^{(N)}(z) - \mathcal{E}_{\nu}^{(\text{exact})}(z) \right|^{2} dz}{\int_{-a}^{a} \left| \mathcal{E}_{\nu}^{(\text{exact})}(z) \right|^{2} dz}}.$$
(3.16)

The results are shown in Fig. 3.8, where we have matched exact and perturbed RS using the MA and plotted Δ_{ν} for different basis sizes N. We see that the trend in accuracy with state number and the basis size is the same as in Fig. 3.4(e),(g), and the RMS deviation versus the normalized state number also shows a universal dependence similar to those in Fig. 3.4(f),(h). However, the EF is in general less well reproduced than the wave numbers and the power law $\Delta_{\nu} \propto (\nu/N)^3$ is observed only in the interval of $0.05 < \Delta_{\nu} < 0.2$.



Figure 3.8: Root mean square deviation of the RS electric field \mathcal{E}_{ν}^{N} from its exact value $\mathcal{E}_{\nu}^{(\text{exact})}$ versus the state number ν (a) and normalized state number ν/n_{max} (b), calculated for different basis sizes N. The straight magenta line in (b) shows a cubic scaling.

3.2.3 Green's function and transmission

The Green's function (GF) is an important quantity which fully characterizes the response of an optical system, determining its scattering and transmission. For the slab with a wide perturbed layer given by Eqs. (3.1) and (3.13), the GF G(z, z'; k)which satisfies the equation

$$\left\{\frac{\partial^2}{\partial z^2} + \left[\varepsilon(z) + \Delta\varepsilon(z)\right]k^2\right\}G(z, z'; k) = \delta(z - z')$$
(3.17)

and outgoing boundary conditions can be calculated analytically. Note that when calculating observables, k is real as it is given by the vacuum wave number of an external driving field. The GF is calculated using its spectral representation, Eq. (2.13)

$$G(z, z'; k) = \sum_{\nu} \frac{\mathcal{E}_{\nu}(z)\mathcal{E}_{\nu}(z')}{2k(k - \varkappa_{\nu})}, \qquad (3.18)$$

in which the EF $\mathcal{E}_{\nu}(z)$ and the RS wave numbers \varkappa_{ν} are calculated numerically via the RSE. For the wave numbers \varkappa_{ν} , we use the extrapolated values Eq. (2.61). In



Figure 3.9: The root mean square deviation in the GF Δ^{GF} as a function of the wave number of the driving field k, calculated via the RSE for different basis sizes N.

light of the importance of the GF and its further usage for calculation of observables, we compare $G^{(N)}$, the GF calculated by RSE with basis size N and Eq. (3.18), to its exact analytic form $G^{(\text{exact})}$, again using the RMS deviation as given by

$$\Delta^{\rm GF} = \sqrt{\frac{\int_{-a}^{a} \int_{-a}^{a} \left| G^{(N)}(z, z') - G^{(\rm exact)}(z, z') \right|^{2} dz dz'}{\int_{-a}^{a} \int_{-a}^{a} \left| G^{(\rm exact)}(z, z') \right|^{2} dz dz'}}.$$
(3.19)

Such a comparison is shown in Fig. 3.9 for different basis sizes N. Increasing the basis size has two effects on the GF: (i) it improves the GF error at a given k and (ii) widens the k-range of the GF with small error. The latter is due to a larger wave-number range of poles in the GF, Eq. (3.18), being reproduced for large N.

Both expansions Eqs. (2.47) and (3.18), for the EF and for the GF, are valid only inside the slab or on its borders and are not suitable for the vacuum area where the EF of the RS grow exponentially. The GF itself is, however, regular on the real k-axis. Moreover, in vacuum, it always has a simple analytic form of a plane wave with the amplitude that can be deduced from values inside the slab, Eq. (3.18), using the continuity of the GF when passing through the interfaces. In this way, the GF can be calculated at any point of the (z, z') space, inside or outside the slab. The δ -function in Eq. (3.17) plays the role of a source of plane waves generated at the



Figure 3.10: (a) Light transmission through the slab with a wide-layer perturbation Eq. (3.13). (b) Absolute error in the transmission calculated using the analytic form of T(k) and numerical values from the RSE for two different simulations.

point z' and propagating in both directions, away from the source. The GF then has the meaning of the system's response to such a plane-wave excitation. This can be used to derive a formula for the transmission in terms of the GF. To do this, we place the source of strength 2ik just outside the slab at z' = -a, in order to produces two plane wave of amplitude 1. One of these waves is transmitted trough the slab, and just after the slab at point z = a the amplitude of the EF (which does not change with further increase of z) is given by

$$T(k) = 2kiG(a, -a; k)$$
(3.20)

and is called transmission.

We calculate the transmission using Eqs. (3.18) and (3.20) for the GF taken to be either numerical $G^{(N)}$ or analytical $G^{(\text{exact})}$. This allows us to calculate the absolute error in the square modulus of transmission, which is shown in Fig. 3.10(b). The transmission itself is shown in Fig. 3.10(a) and has a profile which is fully determined by the pole structure of the GF. The RS which contribute in this frequency range can be seen in the inset to Fig. 2.

3.2.4 δ -perturbation

We now move from a wide perturbation to a very narrow and strong one, like a thin metal film on a dielectric. Such a perturbation is described by

$$\Delta \varepsilon(z) = w \epsilon_d \delta(z - a/2) \tag{3.21}$$

with the δ -scatterer strength $w\epsilon_d = -0.1a$. Physically, this perturbation corresponds to a thin layer of the dielectric constant changed by ϵ_d , which is placed at z = a/2 and has a width w much narrower than the shortest wavelength of the resonant modes used in the basis. The dielectric profile for the system with the δ -perturbation is shown in Fig. 3.11.



Figure 3.11: Dielectric constants of the unperturbed slab $\varepsilon(z)$ and a slab with a δ -perturbation $\varepsilon(z) + \Delta \varepsilon(z)$. The distance z is in units of the half width a of the slab.

As in the case of a wide-layer perturbation considered in Section 3.2.1 we plot and compare in Figs. 11–14 the RS wave numbers, calculated exactly and via the RSE with and without extrapolation, as well as the parameters of the power law fit and



Figure 3.12: As Fig. 3.3 but for the δ -perturbation shown in Fig. 3.11.

relative and absolute errors which we also need for the quality check of the simulation and extrapolation. The analytic solutions for the δ -perturbation and its matrix elements are given in the appendix C. We see in Fig. 3.12 that the extrapolation reduces the relative error by 1-2 orders of magnitude. The integral strength of the perturbation is almost two orders of magnitude weaker than in the case of the wide layer considered in Section 3.2.1. However, the convergence is much slower in the case of the δ -perturbation. We see in Fig. 3.13(c),(d) that for large N the power law exponent is close to $\alpha_{\nu} = -1$. This is to be expected as the δ -perturbation does not have a finite width. The matrix elements V_{nm} , though oscillating do not decrease with increasing wave number (or index n) which leads to a much stronger mixing of states compared to the wide layer perturbation. Indeed, in the wide layer case, states with higher indices are less important due to the rapid oscillation of their wave functions, so that the matrix elements scale as $V_{nm} \propto 1/n$ (for $n \gg m$). Using the second-order Rayleigh-Schrödinger perturbation theory and the explicit form Eqs. (C.6) and (C.8)of the matrix elements V_{nm} , we show that the wave number corrections scale as 1/Nand $1/N^3$ for the δ - and wide-layer perturbations, respectively, in accordance with



Figure 3.13: As Fig. 3.4 but for the δ -perturbation shown in Fig. 3.11. The horizontal magenta lines in panels (c) and (d) are $\alpha = -1$ lines.

Figs. 3(d) and 12(d).

In the case of the δ -perturbation, the absolute errors shown in Fig. 3.13(f,h) as functions of the normalized state number do not display universal curves, for small ν/N is approaching asymptotically a cubic law in the state number ν (magenta lines). Thus we conclude that in this case $M_{\nu} \propto \nu^3/N$ [compare with Eq. (3.14)]. At larger values of ν/N this dependence transforms into a linear one, $M_{\nu} \propto \nu/N$ (blue lines). Because of the slow (1/N) convergence, the extrapolation gives a huge improvement as is clear from Fig. 3.14 and demonstrates its necessity in the particular case of the δ perturbation. At the same time, the relative extrapolation error is predicted within an



Figure 3.14: As Fig. 3.5 but for the δ -perturbation shown in Fig. 10 and state number $\nu = 28$.

order of magnitude, as can be seen in Fig. 3.15. For the majority of RS, $F_{\nu}^{(\text{exact})} < F_{\nu}$, the exact values $F_{\nu}^{(\text{exact})}$ being significantly overestimated. However, for a large class of solutions it turns out to be highly underestimated. The systematic deviation seen Fig. 3.15 in estimating the relative extrapolation error though F_{ν} may be a result of the systematic variation in the power law exponent α_{ν} well seen in Fig. 3.13(c),(d). Hence it is generally advisable when studying convergence with our method to run simulations with a variety of N_4 parameters in order to establish over what range of N_4 the power law is applicable for the given strength of perturbation. We were also able to



Figure 3.15: As Fig. 5, but for the δ -perturbation shown in Fig. 10.

simulate a δ -perturbation outside the perturbed slab by taking the unperturbed slab to include the position of the delta scatterer and thus the perturbation consisting of a superposition of a δ -perturbation and a wide layer compensating the difference in the dielectric constants between the vacuum and the unperturbed slab. In this case we did obtain convergence of the perturbed wave numbers to the exact solution. However, for a δ -perturbation outside of the unperturbed slab or exactly on the border, the simulation does not converge to the correct solution. This is to be expected since in this case the perturbed RS contain waves reflected from the external perturbation, which are waves propagating towards the slab. Such incoming waves are not part of the basis of unperturbed RS, and thus cannot be reproduced by an expansion in this basis.

3.2.5 MICROCAVITY

To evaluate the RSE in presence of sharp resonances, we use a Bragg-mirror microcavity (MC), which consists of a Fabry-Pérot cavity of thickness L_C and refractive index n_C surrounded by distributed Bragg reflectors (DBRs). The DBRs consist of P pairs of dielectric layers with alternating high ($n_H = 3.0$) and low ($n_L = 1.5$) refractive index. In order to have a sharp cavity mode at a given wavelength λ_C , these alternating layers have to be of quarter wavelength optical thickness, and the optical thickness of the cavity has to be a multiple of half the wavelength. We take $L_C = \lambda_C/2$. An example of the dielectric profile of such a system with P = 3 is shown in Fig. 3.16. The RS of a MC are calculated using the RSE. The RS wave vectors



Figure 3.16: Dielectric profiles of a planar microcavity having P = 3 pairs of Bragg mirrors on each side (blue line) and an unperturbed dielectric slab (orange line).

and the transmission through the MC are shown in Fig. 3.17(a),(b). For reference, the unperturbed eigenvalues are also included in Fig. 3.17(a). The unperturbed system taken for the RSE is again a dielectric slab whose dielectric constant $\varepsilon(z)$ can be seen in Fig. 3.16. Throughout this section the outer boundaries of the MC and the unperturbed slab coincide, and we choose $\epsilon_s = 5.5$ which is between n_L^2 and n_H^2 , providing good convergence. In order to verify the transmission calculated by the RSE,



Figure 3.17: (a) Wave vectors \varkappa_{ν} of the resonant states of a microcavity with P = 3 pairs of Bragg mirrors on each side calculated via RSE with N = 801. (b) Microcavity transmission as a function of the normalized wave vector of the incoming light; L_C and n_C are the cavity thickness and refractive index. (c) The difference in the transmission calculated via RSE and using the scattering matrix method [34].



Figure 3.18: The FWHM (a) and the position of the cavity mode (b) calculated analytically and via the RSE for different number of pairs P of Bragg mirrors on each side of the microcavity. N is the basis size used in the RSE. Where possible, extrapolated wave numbers have been used. Crossed symbols for N = 51 indicate states which are rejected by the SC.

we use the scattering matrix method [34] which is a straightforward and precise way of calculating the optical properties of a planar system. Figure 3.17(c) demonstrates a good agreement between the two calculations.

Clearly, there is a one-to-one correspondence between the RS wave vectors in Fig. 3.17(a) and the MC transmission in Fig. 3.17(b). Namely, the real part of the wave vectors corresponds to the positions of the peaks in the transmission while the imaginary part gives their line widths. This is well understood in view of the spectral representation of the Green's function Eq. (3.18) used for the calculation of the transmission via Eq. (3.20).

One of the modes shown in Fig. 3.17(a) is rather isolated and has imaginary part much smaller than the others. This mode, \varkappa_C , satisfies the Fabry-Pérot resonance condition $\operatorname{Re} \varkappa_C = \pi/(L_C n_C)$ and is called the cavity mode. For the wave vector k of incoming light close to this resonance condition, $k \approx \pi/(L_C n_C)$, the Greens' function Eq. (3.18) is dominated by a single term corresponding to this narrow mode. As a consequence, there is a sharp peak in the center of a wide stop-band seen in the transmission in Fig. 3.17(b). For sufficiently large P an analytic approximation for its full width at half maximum (FWHM) of the square modulus of T(k)is known [35],

$$\Delta k = \frac{4n_{\text{ext}}}{n_C^2} \left(\frac{n_L}{n_H}\right)^{2P} \frac{1}{L_C + \frac{\lambda_C}{2} \frac{n_L n_H}{n_C (n_H - n_L)}},$$
(3.22)

which we use to compare with the RSE calculation. With the refractive index of the external material $n_{\text{ext}} = 1$ and using $\lambda_C = 2L_C$ and $n_C = n_H$, Eq. (3.22) reduces to $\Delta k = 4(n_H - n_L)(n_L/n_H)^{2P}/(L_C n_H^3)$. Comparison of the above formula with the RSE result for the cavity mode is given in Fig. 3.18, for different number of Bragg-mirror pairs P and for different basis size N in the RSE. Figure 3.18 demonstrates that RSE is capable of giving both the correct width and location of sharp resonances in the transmission profile, if a large enough basis is used, in spite of there being no sharp resonances in the basis. As the basis size is enlarged, the width and the peak location of the cavity mode converge to the analytic values. The fact that for a fixed N the cavity mode position and the width are predicted worse for larger P is explained by our choice of the unperturbed slab which always has exactly the same thickness as the Bragg-mirror MC. With the number of Bragg-mirrors increasing, the field inside the MC oscillates more rapidly (also shifting the cavity mode towards higher frequencies) that requires a larger number of RS to be taken into account in order to produce results on the same level of accuracy. We have verified (not shown) that the errors become independent of P, if one and the same constant width of the unperturbed slab is used for different values of P.

3.3 ROLE OF WAVEGUIDE MODES IN TRANSMISSION SPEC-TRA

In this section we will report the study of planar electrodynamic systems with non-zero in-plane momentum by calculating the contribution in the Mittag-Leffler expansion from different types of modes to the transmission. It is shown that the WG modes have a finite contribution to the transmission due to off resonance excitation.

For the RSs given in Sec. 3.1, we calculate from Maxwell's BCs that for the region z > a the electric field for the transmitted plane wave is given by $E(z) = t(\omega)e^{ikz}E_0$ where E_0 is the amplitude of the incoming wave. The field transmission through the slab $t(\omega)$ has the analytic form

$$t(\omega) = \frac{2ikqe^{-2ika}}{2ikq\cos(2qa) + (k^2 + q^2)\sin(2qa)} = T(k),$$
(3.23)

in which

$$k = \sqrt{\left(\frac{\omega}{c}\right)^2 - p^2}, \qquad (3.24)$$

$$q = \sqrt{\epsilon_s \left(\frac{\omega}{c}\right)^2 - p^2} = \sqrt{\epsilon_s k^2 + (\epsilon_s - 1)p^2}$$
(3.25)

are the z-components of the wave vector in vacuum and dielectric, respectively. Eq. (3.23) shows that the transmission $t(\omega)$ is a function of the real frequency ω . We can also express the transmission $t(\omega)$ as a function T(k) of the normal wave vector k, in which k takes only real positive values, as dictated by the outgoing character of the transmitted wave. The wave vector q inside the slab can be complex for a dielectric with dissipation and have an arbitrary sign, reflecting the fact that waves within the slab propagate in both directions. Hence the transmission is insensitive to the sign of q as seen in Eq. (3.23).

To study the influence of different modes on the transmission, we consider analytic continuations (ACs) $\tilde{t}(\omega)$ and $\tilde{T}(k)$ of both functions in the complex ω - and k-plane, respectively, in order to investigate their pole structure and for each of them apply the Mittag-Leffler theorem [30, 36]. The AC of the transmission has different types of poles, which are shown in Fig. 3.1 for pa = 5 and discussed in Sec. 3.1. The function $\tilde{t}(\omega)$ has two branch points at $\omega = \pm pc$ connected by a cut, due to the square root in Eq. (3.24). We choose the cut going through $\omega = -i\infty$ and thus producing two vertical cut lines as shown in Fig. 3.1. The other square root in the definition of $q(\omega)$ does not produce any cuts due to the above mentioned fact that $t(\omega)$ is an even function of q and thus independent of its sign. Integrating $\tilde{t}(\omega')/(\omega - \omega')$ over a closed infinite-radius circular contour circumventing the cut, similar to that used in Ref.[37], we obtain the spectral representation in the frequency domain

$$\tilde{t}(\omega) = \sum_{n} \frac{\operatorname{Res}_{\omega'=\omega_{n}} \left[\tilde{t}(\omega')\right]}{\omega - \omega_{n}} + \frac{1}{2\pi i} \sum_{p'=\pm p} \int_{p'c-i\infty}^{p'c} \frac{\Delta t(\omega')d\omega'}{\omega - \omega'}.$$
(3.26)

Here the first term represents a sum over residues at all poles of $\tilde{t}(\omega)$. The second term is the integral of the step $\Delta t(\omega)$ in the transmission along the two parts of the cut shown in Fig. 3.1. Specifically, $\Delta t(\omega)$ is defined as the difference between the values of $\tilde{t}(\omega)$ on the left and right sides of the cut for the given cut point ω .

Using the spectral representation Eq. (3.26) for real frequencies ω , we analyse contributions of the poles and the cut to the transmission. The transmission is usually studied for a fixed angle of incidence θ , motivated by experimental constraints. An example of the calculated transmission through a slab with $\epsilon_s = 9$ is shown for $\theta = \pi/4$ in Fig. 3.19 (a). For a fixed θ , the in-plane wave vector p changes with frequency, so that the contributions of the poles (which are different for different p) are not constant across the spectrum. Therefore analysis of the spectrum for a fixed p is made, as shown in Fig. 3.19 (b), in which the contributions of different pole types and the cut are shown individually, summing up to the analytic transmission Eq. (3.23). Note that the transmission $t(\omega)$ is defined over the angle range $0 < \theta < \pi/2$, corresponding to $\omega > pc$. FP modes dominate for $\omega \gg pc$ giving rise to the oscillations in the transmission, while the contribution of all other modes and the cut are significant only close to the threshold $\omega = pc$, corresponding to grazing incidence $\theta \sim \pi/2$.

The cut contribution to the spectral representation Eq. (2.40) and to the transmission in Fig. 3.19 (b) produces a continuum of resonances. Such a continuum can be approximately treated in the RSE by replacing it with a series of poles, as we did in Ref.[37]. In the present case however, the cut can actually be removed by going into the wave-vector domain. Indeed, being treated as a function of the normal wave vector k, the AC of the transmission $\tilde{T}(k)$ has no cuts in the complex k-plane



Figure 3.19: Transmission $|t(\omega)|$ of a homogeneous dielectric slab with $\epsilon_s = 9$ as a function of the light frequency ω , (a) for a fixed angle of incidence $\theta = \pi/4$ and (b) for a fixed in-plane wave vector pa = 5, along with partial contributions to the transmission of different types of modes and the cut shown in Fig. 3.1. Black vertical arrows indicate the frequency for which pa = 5 in panel (a) and $\theta = \pi/4$ in panel (b). The inset shows a schematic of the total wave vector ω/c along with its projections p and k on the x- and z-axis, respectively.



Figure 3.20: Transmission |T(k)| of a homogeneous dielectric slab with $\epsilon_s = 9$ and pa = 5 and partial contributions of different modes, as functions of the normal component of the wave vector in vacuum k. As in Fig. 3.19 (b), vertical arrows indicate the wave vector at which $\theta = \pi/4$.

and its spectral representation obtained by using the Mittag-Leffler theorem has the following form:

$$\tilde{T}(k) = \sum_{n} \frac{\operatorname{Res}_{k'=k_n} \left[\tilde{T}(k') \right]}{k - k_n}, \qquad (3.27)$$

in which $k_n = \sqrt{\omega_n^2/c^2 - p^2}$, with *n* numbering the poles as in Eq. (2.40). On the real k-axis, $\tilde{T}(k)$ coincides with the transmission T(k) given by Eq. (3.23) and is shown in Fig. 3.20 along with the contributions of the different types of modes. We see in particular that the WG modes, which are not emitting into an outgoing plane wave, and thus by reciprocity are expected not to be excitable by an incoming plane wave, have a finite contribution to the transmission, which is possible only due to their off-resonant excitation. This contribution increases with decreasing the wave vector k, as the frequency of the incoming wave is getting closer to the resonant frequencies of the WG modes lying beyond the vacuum light cone.

3.4 NUMERICAL RESULTS FOR NON-NORMAL INCIDENCE

In this section results of the RSE for an electrodynamic system with non-zero in-plane momentum are reported. We make use of exact solutions which are available for these simple geometries to prove the accuracy of the numerical calculations required in the RSE so as to justify further development of the method in subsequent chapters of this thesis.

We find the perturbed modes by solving the linear matrix problem given by Eq. (2.34). The matrix elements V_{nm} are given by

$$V_{nm} = \int_{-a}^{a} \Delta \varepsilon(z) E_n(z) E_m(z) dz , \qquad (3.28)$$

where E_n are given in Eq. (3.5).

3.4.1 UNPERTURBED RESONANT STATES

The frequencies ω_n of the RSs of a dielectric slab for pa = 5 and $\epsilon_s = 9$ were shown in Fig. 3.1. The normal wave vectors k_n of the RSs for a slab with $\epsilon_s = 3$ versus p are given in Fig. 3.21. All states in the range $|\text{Re }k_na| < 5$ and $|\text{Im }k_na| < 5$ for |pa| < 5 are shown in Fig. 3.21 (a) and separated into mode types in Fig. 3.21 (b) and (c). For WG and AWG modes $\text{Re }k_n = 0$, therefore Fig. 3.21 (c) shows only their imaginary part, which is positive for WG modes, corresponding to evanescent waves, and negative for AWG modes, corresponding to exponentially growing waves outside the slab. The WG and AWG modes continuously transform into each other and produce branches similar to those seen also for FP modes. These branches cross each other at certain points [shown in Figs. 3.21 (b) and (c) by magenta dots] where two FP modes are transformed into two AWG modes. The AWG mode branch which starts at p = 0 has no connection to any WG or FP branches; a mode on this branch was identified in Fig. 3.1 as the leaky mode.

The RSs of the homogeneous slab shown, similar to those shown in Fig. 3.21, are used as a basis for the RSE in the two examples given next. In general, for any local perturbation $\Delta \varepsilon(z)$ which does not change the translational symmetry of the



Figure 3.21: Resonant state wave numbers of a homogenous dielectric slab with $\epsilon_s = 3$ as function of the in-plane wave vector p: (a) The complex wave vectors k_n of Fabry-Perot (red lines) and WG and AWG modes (black lines), with a projection on the lower plane; (b) Re k_n of Fabry-Perot modes with the color giving the value of Im k_n ; (c) Im k_n of the WG and AWG modes. The points where the modes in panels (b) and (c) connect are given by magenta dots joined by dashed lines.

slab, i.e. does not depend on x or y, the in-plane momentum p remains a good quantum number. In other words, $\Delta \varepsilon(z)$ does not mix states with different p, so that in any such problem solved by the RSE, we can use the basis of RSs with a given fixed value of p.

3.4.2 Full-width perturbation

To illustrate the accuracy and convergence of the RSE, we consider a homogeneous full-width perturbation of the slab, which is given by

$$\Delta \varepsilon(z) = \begin{cases} \Delta \epsilon & \text{for } |z| \leq a, \\ 0 & \text{otherwise}, \end{cases}$$
(3.29)

and for which the exact solution can be obtained by solving the transcendental Eq. (3.6) with ϵ_s replaced by $\epsilon_s + \Delta \epsilon$. We denote these exact perturbed wave numbers as $\varkappa_{\nu}^{(\text{exact})}$ and compare them with the perturbed values \varkappa_{ν} obtained by using the RSE for different basis sizes N. We choose as basis of given size all poles with $|k_n| < k_{\max}(N)$, using a suitably chosen wave-number cutoff $k_{\max}(N)$.

In Fig. 3.22 we compare the RSE wave numbers with the exact wave numbers for our system in the case of pa = 5. We can see in Fig. 3.22(a) that the RSE is reproducing the exact solution to a high accuracy, which is quantified by the relative error $|\varkappa_{\nu}/\varkappa_{\nu}^{(\text{exact})} - 1|$ shown in Fig. 3.22(b) for the FP modes with Re $\varkappa_{\nu} > 0$ and in Fig. 3.22 (c) for the WG and AWG modes. We see that the relative error scales as N^{-3} . We find in the simulation used to generate Fig. 3.22 for a basis of N = 2000 that the RSE reproduces about 300 modes with a relative error below 10^{-8} . This error can be further improved by 1-2 orders of magnitude using the extrapolation method described in Section 2.4.

3.4.3 MICROCAVITY PERTURBATION

To evaluate the RSE for inclined geometry in the presence of sharp resonances in the optical spectrum, we use a Bragg-mirror MC, which consists of a FP cavity of



Figure 3.22: (a) Exact (squares) and calculated by the RSE with N = 2000 (crosses) resonant state wave numbers of a homogeneous dielectric slab with $\epsilon_s = 3$ along with those of the unperturbed slab with $\epsilon_s = 9$ (circles with a dot). Relative errors in calculation of Fabry-Perot modes (b) and waveguide and anti-waveguide modes (c) for different total number of basis states N used in the RSE as labeled. Inset: the dielectric constant profile of the unperturbed and perturbed systems, with the full-width homogeneous perturbation of the slab $\Delta \epsilon = -6$.

thickness $L_{\rm C}$ and dielectric constant $\epsilon_{C} = 9$ surrounded by distributed Bragg reflectors (DBRs). The DBRs consist of P = 5 pairs of dielectric layers with alternating high $\epsilon_{H} = 9$ and low $\epsilon_{L} = 2.25$ susceptibility, as illustrated by the inset in Fig. 3.23. The alternating layers have a quarter-wavelength optical thickness and the cavity has a half-wavelength optical thickness. The nominal wavelength which determines the layer thickness is that of the lowest-frequency CM at normal incidence. As unperturbed system we used a dielectric slab with $\epsilon_s = 9$ as in Sec. 3.4.2.



Figure 3.23: (a) The same as in Fig. 3.22 (a) but with the perturbed system being the Bragg-mirror microcavity with the dielectric profile shown in the inset. The lowest-energy cavity mode is shown by an arrow. (b) Transmission as a function of the normal component of the wave vector k, for the perturbed (thick black curve) and unperturbed system (thin red curve) demonstrating the correspondence between the RS wave numbers in panel (a) and peaks in the transmission.

The unperturbed modes of the slab and the perturbed modes of the MC are

shown in Fig. 3.23 (a) for pa = 5. We can see how the nearly equidistant FP modes of the unperturbed system are redistributed in the MC, transforming into a sharp CM in the middle of a wide stop-band and modes outside of the stop-band. The link between the peaks in the transmission in Fig. 3.23 (b) and the poles in Fig. 3.23 (a) is also exemplified by the real part of the poles giving the position of the peaks in transmission and the imaginary part giving their linewidth. This is discussed in Sec. 3.2.5 where transmission is defined in Eq. (3.20).



Figure 3.24: The same as in Fig. 3.21 (b) but for the Bragg-mirror microcavity with the dielectric profile given by the inset in Fig. 3.23 (a).

The transmission T(k) for a layered planar structure can be calculated using the transfer matrix method leading to the explicit result

$$T(k) = \frac{e^{-i(q_0+q_M)a}}{\xi_M^+}, \qquad (3.30)$$

in which ξ_M^+ is found from the recursive formula

$$2\xi_{j+1}^{\pm} = \left(1 \pm \frac{q_{j+1}}{q_j}\right) e^{-iq_j a_j} \xi_j^+ + \left(1 \mp \frac{q_{j+1}}{q_j}\right) e^{iq_j a_j} \xi_j^-$$
(3.31)

with the starting value

$$2\xi_1^{\pm} = \left(1 \pm \frac{q_1}{q_0}\right) \tag{3.32}$$

and the normal component of the wave vector in the j-th layer

$$q_j = \sqrt{\epsilon_j k^2 + (\epsilon_j - 1)p^2}.$$
(3.33)

Here ϵ_j and a_j are, respectively, the dielectric constant of the *j*-th layer and its width, so that $\sum_{j=1}^{M-1} a_j = 2a$. The layers j = 0 and j = M correspond to the vacuum before and after the MC, respectively, so that $q_0 = q_M = k$, and $q_j \ge 0$ for real ϵ_j . M gives the total number of interfaces in the structure, in the present case M = 2(2P + 1).

In Fig. 3.24 we show the evolution of the perturbed poles with p. We see that one of the modes is separated in the middle of a gap and has an imaginary part well below the others. This mode is known as the CM. The perturbed Green's function which has a spectral representation equivalent to Eq. (2.44) and the corresponding transmission T(k) are dominated by the single term from the CM in this frequency region, therefore a sharp isolated peak is seen in the center of the stop-band in Fig. 3.23 (b). Interestingly, the modes in Fig. 3.24 show an almost circular behavior, indicating that the frequency of each mode $\omega_{\nu} = c\sqrt{\varkappa_{\nu}^2 + p^2}$ is approximately constant versus angle θ .

Indeed, we can see in Fig. 3.25 (a) that the CM frequency ω_C has a weak dependence on θ , while the corresponding wave vector \varkappa_C changes more strongly. In parallel, the linewidth given in Fig. 3.25 (b) shows a similar behavior both in the ω -and k-representations, though at $\theta \to \pi/2$ the imaginary part of ω_C is one order of magnitude smaller than that of \varkappa_C .

Figures 3.25(a) and (b) demonstrate a good agreement between \varkappa_C obtained using the RSE and $\varkappa_C^{(\text{exact})}$ extracted from the linewidth in the transmission calculated via Eqs. (3.30)–(3.33). Fig. 3.25(c) shows the relative error $|\varkappa_C/\varkappa_C^{(\text{exact})} - 1|$ for different values of N demonstrating convergence of the RSE for the cavity mode with N^{-3} , the same as for the homogeneous perturbation of the slab. The convergence behavior depends on the distribution of the perturbation in the wave-vector space as


Figure 3.25: Real (a) and imaginary part (b) of the cavity mode frequency ω_C (left axes) and normal component of the wave vector \varkappa_C (right axes) calculated using the RSE (blue crosses) for N = 2000, the transfer matrix method (red circles and open squares) and the analytic approximation Eq. (3.34) for the linewidth $\Gamma = -\text{Im} \omega_C$ (green open circles). (c) Relative error of \varkappa_C determined by RSE for different basis sizes N as given. All data are shown as a function of the angle of incidence θ , and all symbols are connected by lines as a guide to the eye.

discussed in Sec. 3.2. Interestingly, the RSE can reproduce sharp resonances in the transmission profile, in spite of the absence of sharp resonances in the basis.

We also compare the results in Fig. 3.25(b) with an analytic approximation for the CM linewidth

$$\operatorname{Im}\omega_{C} = -\frac{2c\eta_{\text{ext}}}{n_{C}\eta_{C}} \frac{\left(\eta_{L}/\eta_{H}\right)^{2P}}{L_{C}\cos(\theta_{C}) + \frac{\lambda_{C}}{2}\frac{\eta_{L}\eta_{H}}{\eta_{H} - \eta_{L}}\frac{1}{\eta_{C}}},$$
(3.34)

which was derived by generalizing the approximation for normal incidence of light available in the literature [35, 38, 39]. Here n_j is the refractive index of layer j, $\eta_j = n_j \cos(\theta_j)$, and θ_j is the angle to the normal in layer j, given by $\sin(\theta_j)n_j = n_{ext}\sin(\theta)$. The layers j used are: the external region (ext) which is vacuum in our case, the highindex (H) layer, the low-index (L) layer of the Bragg mirror, and the cavity layer (C). The cavity wavelength is given by $\lambda_C = 2L_C\cos(\theta_C)$. Equation (3.34) is exact in the limit $P \to \infty$, for a structure with Bragg-mirror layer widths strictly equal to a quarter-wavelength and the cavity layer width to a half-wavelength optical thickness. This condition depends on the incident angle, and in our fixed structure is fulfilled for normal incidence only. Nevertheless, Eq. (3.34) reproduces the exact result reasonably well over the whole angle range, as shown in Fig. 3.25(b).

3.5 SUMMARY

The resonant state expansion has been implemented and validated in planar open optical systems which represent effective one-dimensional systems. A reliable method of calculation of resonant states, and in particular their wave numbers, electric fields, as well as the Green's function and the transmission of such systems, has been developed and demonstrated. It includes estimation of the accuracy and convergency of calculations and in particular extrapolation of the RS-wavevectors towards their exact values which are generally not available. Particular examples which illustrate the general method and the developed algorithm include a dielectric slab with widelayer and δ -perturbations as well as an optical microcavity using Bragg mirrors. In these examples, a comparison with exact solutions has been made in order to verify the approach. In all three systems the resonant states and the transmission are calculated to any required accuracy by the resonant state expansion. The extrapolation of the wave vectors using the power law in the basis size, which has been developed and demonstrated, significantly improve the accuracy of calculations, by one or two orders of magnitude.

The RSE has also been generalized to planar optical systems with inclined geometry. In inclined geometry, the spectrum of a planar system contains a continuum of resonances originating from a cut of the Green's function, which we have eliminated by mapping the frequency into the normal component of the wave vector. The optical modes and spectra of a perturbed planar system are then calculated by solving a linear matrix eigenvalue problem containing matrix elements of the perturbation in the basis of discrete resonant states only. We have verified the method on full-width homogeneous and Bragg-mirror microcavity perturbations and compared results with obtained analytic solutions, demonstrating fast convergence of the method towards the exact result. We expect that it will be possible to extend this treatment to inclined geometries that are effectively two-dimensional using a similar approach, which would provide an efficient algorithm to calculate the optical modes in fibers and waveguides, including photonic crystal fibers having a complex structure.

By examining the transmission using the Mittag-Leffer theorem it was seen that the WG modes, which are not emitting into an outgoing plane wave, and thus by reciprocity are expected not to be excitable by an incoming plane wave, have a finite contribution to the transmission, which is possible only due to their of- resonant excitation. This contribution increases with decreasing the wave vector, as the frequency of the incoming wave is getting closer to the resonant frequencies of the WG modes lying beyond the vacuum light cone.

Chapter 4

RSE applied to two-dimensional open optical systems

In this chapter we apply the RSE method to effectively two-dimensional (2D) systems (i.e. 3D systems translational invariant in one dimension) which are *not reducible* to effective 1D systems. We limit the treatment to systems with zero wavevector projection along the translational invariant direction. We use a dielectric cylinder with uniform dielectric constant in vacuum as the unperturbed system and calculate the perturbed RSs for homogeneous (i.e. reducible to 1D) and inhomogeneous perturbations, including a half-cylinder, thin-film, and thin-wire perturbation. None of these inhomogeneous perturbations have known exact analytic solutions which could be used for verification of the RSE. However, the case of a narrow wire inside a cylinder allows for an approximate analytic solution suitable for weak perturbations [40, 41]. This solution is compared with the present results of the RSE, demonstrating a good agreement.

One striking feature of 2D systems, which we reveal in this chapter, is the presence of a one-dimensional continuum in the manifold of RSs. This continuum is specific to 2D systems and is required for the completeness of the basis and thus for the accuracy of the RSE applied in 2D as discussed below in some detail. Such continua are generally known in the theory of quasi-guided modes in photonic crystal structures [42] as potential sources of Wood-Rayleigh anomalies in optical spectra [43– 47]. These continua are similar to those in planar structure with $p \neq 0$. Technically, they are caused in that case by the presence of square roots in the photon dispersion of light propagated and Bragg scattered inside the photonic crystal just as in the case of a planar structure with $p \neq 0$. In the case of a dielectric cylinder, which is used for the RSE in 2D, the continuum originates mathematically from the cut in the cylindrical Hankel functions solving Maxwell's equations outside the cylinder.

The spectral representation of the 2D system GF is modified to include this cut contribution as the integral:

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\mathbf{E}_{n}(\mathbf{r}) \otimes \mathbf{E}_{n}(\mathbf{r}')}{2k(k-k_{n})} \approx \sum_{\bar{n}} \frac{\phi_{\bar{n}} \mathbf{E}_{\bar{n}}(\mathbf{r}) \otimes \mathbf{E}_{\bar{n}}(\mathbf{r}')}{2k(k-k_{n})}.$$
(4.1)

In practice, the continuum of non-resonant states is discretised and included as cut poles in the perturbation basis. We treat this problem in detail in Sec. 4.1. The combined index \bar{n} is used to denote both real poles k_n and cut poles k_{α} simultaneously. The weighting factors $\phi_{\bar{n}}$ are defined as follows

$$\phi_{\bar{n}} = \begin{cases} \phi_n = 1 & \text{for real poles,} \\ \phi_\alpha & \text{for cut poles,} \end{cases}$$
(4.2)

After modifying the expansion of the perturbed wave functions to include the cut poles,

$$\boldsymbol{\mathcal{E}}_{\nu}(\mathbf{r}) = \sum_{\bar{n}} \phi_{\bar{n}} b_{\bar{n}\nu} \mathbf{E}_{\bar{n}}(\mathbf{r}) , \qquad (4.3)$$

we can repeat the derivation of Sec. 2.2 to arrive at the modified the RSE Matrix equations,

$$\varkappa_{\nu} \sum_{\bar{n}'} \left(\delta_{\bar{n}\bar{n}'} + \sqrt{\phi_{\bar{n}}\phi_{\bar{n}}'} V_{\bar{n}\bar{n}'}/2 \right) b_{\bar{n}'\nu} = k_n b_{\bar{n}\nu} \,, \tag{4.4}$$

and

$$\sum_{\bar{n}'} \left(\frac{\delta_{\bar{n}\bar{n}'}}{k_{\bar{n}'}} + \frac{V_{\bar{n}\bar{n}'}}{2} \sqrt{\frac{\phi_{\bar{n}}\phi_{\bar{n}}'}{k_{\bar{n}}k_{\bar{n}'}}} \right) c_{\bar{n}'\nu} = \frac{1}{\varkappa_{\nu}} c_{\bar{n}\nu} , \qquad (4.5)$$

As always $V_{\bar{n}\bar{n}'}$ is given by

$$V_{\bar{n}\bar{n}'} = \int \mathbf{E}_{\bar{n}}(\mathbf{r}) \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_{\bar{n}'}(\mathbf{r}) \, d\mathbf{r} \,. \tag{4.6}$$

This chapter is organized as follows. In Sec. 4.1 we treat the homogeneous dielectric cylinder as the unperturbed system. In Sec. 4.1.1 we detail challenges of calculating the cut poles in the 2D TE polarisation and outline the solution to these problems. We add the contribution of the cut in Sec. 4.1.3. This is followed by examples in Sec. 4.2 illustrating the method and comparing results with existing analytic solutions where they are available. We give details of the general formulation of the method in 2D, its application, and the calculation of matrix elements for specific perturbations in Appendices D, E, and F.

4.1 EIGENMODES OF A DIELECTRIC CYLINDER AS BASIS FOR THE RSE

We consider systems in 3D space which are homogeneous in one direction (along the unit vector $\hat{\mathbf{z}}$ of the z-axis), and thus can be reduced to effective 2D systems, as their wavevector component along $\hat{\mathbf{z}}$ is conserved and the solution can be separated into a plane wave $\exp(ik_z z)$ and the remaining (x, y)-problem which we express below in polar coordinates $\boldsymbol{\rho} = (\rho, \varphi)$. For such a system, the solutions of Maxwell's equations split into two groups with orthogonal polarizations, called transverse electric (TE) and transverse magnetic (TM), where TE (TM) states have a electric (magnetic) field orthogonal to $\hat{\mathbf{z}}$. This nomenclature relates to the theory of waveguides where the light propagating along $\hat{\mathbf{z}}$ has the dominant component k_z of the wave vector, and the electric (magnetic) field in TE (TM) modes is thus approximately perpendicular to the wave vector. Although we restrict our treatment here to the limit of $k_z = 0$, we follow these adopted notations. In this case, however, the TE (TM) states have the magnetic (electric) field polarization vector strictly parallel to $\hat{\mathbf{z}}$ and thus normal to the wave vector of light.

4.1.1 MAXWELL'S WAVE EQUATION FOR MAGNETIC FIELD

If we examine Maxwell's wave equation for magnetic field $\mathbf{H}(\mathbf{r})$,

$$-\nabla \times \nabla \times \mathbf{H}(\mathbf{r}) + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times (\nabla \times \mathbf{H}(\mathbf{r})) + k^2 \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{H}(\mathbf{r})$$
$$= -\nabla \times \mathbf{J}(\mathbf{r}) + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times \mathbf{J}(\mathbf{r}), \quad (4.7)$$

it would at first sight seem of no use to the RSE. In Eq. (4.7) we can see $\nabla \hat{\varepsilon}(\mathbf{r})$ which has prevented us from formulating an equation similar to Eq. (2.31) relating the perturbed eigenmodes of magnetic field to their unperturbed GF and perturbation in the dielectric profile. Therefore as we are considering perturbations in the dielectric profile we are forced to formulate the RSE in terms of electric modes $\mathbf{E}_{\bar{n}}(\mathbf{r})$ as previously in Sec. 2.2.

However even in light of the previous paragraph we do need to consider Eq. (4.7) in this chapter because the cut poles cannot be normalised using Eq. (2.23). The method of normalisation will thus make use of Eq. (4.7). The reason we cannot use Eq. (2.23) for the cut poles is that they are not true resonances of the system. This problem can be intuitively understood if we assume we can normalise a single cut pole with Eq. (2.23) and observe the resulting logical contradiction. If the discretisation of the cut is made finer by increasing the number of cut poles by several orders of magnitude, logically the normalisation of the chosen cut pole should be drastically reduced as its weight is further shared between many of these extra poles. This final remark gives the contradiction because the normalisation calculated from Eq. (2.23)

In light of the problems of normalising cut poles we are forced to normalise the basis modes in this chapter by comparing spectral GFs of the form Eq. (2.13) which will still hold true for cut poles, with the analytic GF of the electric or magnetic field calculated in Appendix E. This causes a problem because unlike the TM case where the analytic GF for the electric field $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r'})$ is available, we can only derive the analytic GF for the magnetic field $\hat{\mathbf{G}}_k^{\mathrm{H}}(\mathbf{r}, \mathbf{r'})$ in the case of transverse electric (TE) polarisation. The reason for this is that a scalar GF equation is available for $\hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')$ but not for $\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}')$ in the TE case. However in Appendix D we have been able to derive a method of expressing the electric field basis modes $\mathbf{E}_{\bar{n}}$ in terms of the magnetic field basis modes $\bar{\mathbf{H}}_{\bar{n}}$.

The Green's function for the magnetic component of an electrodynamic system is a tensor $\hat{\mathbf{G}}_k^{\mathrm{H}}$ which satisfies the outgoing wave boundary conditions and Maxwell's wave equation with a delta function source term

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times (\nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')) + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')$$
$$= \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}') . \quad (4.8)$$

Following the derivation for the spectral representation of $\hat{\mathbf{G}}_k$ in Appendix B we find $\hat{\mathbf{G}}_k^{\mathrm{H}}$ can be written as

$$\hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\phi_{\bar{n}} \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}) \otimes \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}')}{2k(k-k_{\bar{n}})}, \qquad (4.9)$$

where the field $\mathbf{\bar{H}}_{\bar{n}}(\mathbf{r})$ satisfies,

$$-\nabla \times \nabla \times \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}) + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times (\nabla \times \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r})) + k^2 \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}) = 0 \qquad (4.10)$$

with outgoing BCs. In this chapter we will make use of $\overline{\mathbf{H}}_{\bar{n}}$ defined in Eq. (4.8), Eq. (4.9) and Eq. (4.10) to normalise $\mathbf{E}_{\bar{n}}$.

4.1.2 UNPERTURBED BASIS FOR 2D SYSTEMS

In this section we will use the approach outlined in Sec. 4.1.1 to formulate the basis states for both TE, TM polarizations. We also find that for completeness of the basis we must include longitudinal electric modes which are curl free static modes satisfying Maxwell's wave equation for $k_n = 0$. Longitudinal magnetic modes have zero electric field, and since we limit ourselves in this work to perturbations in the dielectric susceptibility only, they are not mixed by the perturbation to other types of modes and are thus ignored in the following.

Splitting off the time dependence $\propto e^{-i\omega t}$ of the electric fields **E** and **D** and

magnetic field **H**, the first pair of Maxwell's equations can be written in the form

$$\nabla \times \mathbf{E} = ik\mathbf{H}, \qquad \nabla \times \mathbf{H} = -ik\mathbf{D} \tag{4.11}$$

where $k = \omega/c$ and $\mathbf{D}(\mathbf{r}) = \hat{\boldsymbol{\varepsilon}}(\mathbf{r})\mathbf{E}(\mathbf{r})$. Combining them leads to Eq. (2.6) for the RSs and to Eq. (2.2) for the corresponding GF. For $k \neq 0$ states the second pair of Maxwell's equations,

$$\nabla \cdot \mathbf{D} = 0 \quad \text{and} \quad \nabla \cdot \mathbf{H} = 0,$$

$$(4.12)$$

is automatically satisfied, since $\nabla \cdot \nabla \times \mathbf{A} = 0$ for all \mathbf{A} . However, if k = 0, it is not guaranteed that solutions of Eq. (4.11) satisfy also Eq. (4.12). The spectrum of the GF given by Eq. (2.13) however includes all modes obeying Eq. (4.11), no matter whether Eq. (4.12) is satisfied or not. One finds that the LE modes actually do not satisfy Eq. (4.12) on the sphere surface, such that Maxwell's boundary condition of continuity of the normal component of \mathbf{D} across the boundary of the dielectric sphere is not fulfilled. The LE modes are therefore just formal solutions of Eq. (2.6) not corresponding to any physical modes of the system. However, they have to be taken into account for the completeness of the basis used in the RSE.

Following Ref.[48] for $k_z = 0$, the three groups of modes of a homogeneous dielectric cylinder can be written as

TM:
$$\mathbf{E} = f\mathbf{e}_z$$
,
TE: $\mathbf{H} = f\mathbf{e}_z$,
LE: $\mathbf{E} = -\nabla f$,

where $f(\mathbf{r})$ is a scalar function satisfying the Helmholtz equation

$$\nabla^2 f + k^2 \varepsilon f = 0, \qquad (4.13)$$

with the dielectric susceptibility of the sphere in vacuum

$$\varepsilon(\rho,\varphi) = \begin{cases} n_r^2 & \text{for } \rho \leqslant R, \\ 1 & \text{for } \rho > R. \end{cases}$$
(4.14)

and

$$f(\mathbf{r}) = R_m(\rho, k_n)\chi_m(\varphi). \qquad (4.15)$$

The angular parts are defined by

$$\chi_m(\varphi) = \begin{cases} \pi^{-1/2} \sin(m\varphi) & \text{if } m < 0, \\ (2\pi)^{-1/2} & \text{if } m = 0, \\ \pi^{-1/2} \cos(m\varphi) & \text{if } m > 0, \end{cases}$$
(4.16)

where there is no m = 0 mode for the TE case. The $\chi_m(\varphi)$ are orthonormal according to

$$\int_{0}^{2\pi} \chi_m(\varphi) \chi_{m'}(\varphi) d\varphi = \delta_{mm'} \,. \tag{4.17}$$

The choice of the wave functions in the form of standing waves Eq. (4.16), instead of $e^{im\varphi}$, is dictated by the orthogonality condition Eq. (2.15), which does not use the complex conjugate.

The radial components satisfy,

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2} + \varepsilon(\rho)k^2\right]R_m(\rho,k) = 0$$
(4.18)

and have the form

$$R_m(\rho,k) = \begin{cases} J_m(n_r k \rho) / J_m(n_r k R) & \text{for } \rho \leqslant R, \\ H_m(k \rho) / H_m(k R) & \text{for } \rho > R, \end{cases}$$
(4.19)

in which $J_m(z)$ and $H_m(z) \equiv H_m^{(1)}(z)$ are, respectively, the cylindrical Bessel and Hankel functions of the first kind.

We treat in this work all polarisations, however only TM and LE polarisations

mix due to the perturbations treated being strictly scalar in dielectric permittivity. If the perturbation resulted in a tensor dielectric profile then all polarisations could mix.

The unperturbed RS wave functions factorize as

TM :
$$\mathbf{E}_{n}(\mathbf{r}) = A^{\text{TM}} R_{m}(\rho, k_{n}) \chi_{m}(\varphi) \mathbf{e}_{z} ,$$

TE : $\mathbf{\bar{H}}_{n}(\mathbf{r}) = A_{m}^{\text{TE}}(k_{n}) R_{m}(\rho, k_{n}) \chi_{m}(\varphi) \mathbf{e}_{z} .$ (4.20)

We normalized the wave functions from the analytic TM (TE) Green's function in Appendix E with normalisation constants A(k)

$$A^{\rm TM} = \frac{1}{R} \sqrt{\frac{2}{n_r^2 - 1}} \,. \tag{4.21}$$

$$A_m^{\rm TE}(k_n) = \sqrt{\frac{2k \left[J_m(n_r k R)\right]^2}{\left(n_r^2 - 1\right) \left[\frac{m^2}{k} \left[J_m(n_r k R)\right]^2 + R^2 k \left[J_m'(n_r k R)\right]^2\right]}}$$
(4.22)

The two boundary conditions at the surface of the cylinder, the continuity of the electric field and its radial derivative, produce a secular equation for the RS wave number eigenvalues k_n , which has the form

$$D_m^{\rm TM}(k_n R) = 0,$$
 (4.23)

$$D_m^{\rm TE}(k_n R) = 0,$$
 (4.24)

where

$$D_m^{\rm TM}(z) = n_r J_m'(n_r z) H_m(z) - J_m(n_r z) H_m'(z) , \qquad (4.25)$$

$$D_m^{\rm TE}(z) = J'_m(n_r z) H_m(z) - n_r J_m(n_r z) H'_m(z) , \qquad (4.26)$$

and $J'_m(z)$ and $H'_m(z)$ are the derivatives of $J_m(z)$ and $H_m(z)$, respectively. Here z represents a complex argument, as opposed to the spatial coordinate used earlier.

In cylindrical coordinates, the electric vector field $\mathbf{E}(\mathbf{r})$ can be written as

$$\mathbf{E}(\rho,\varphi,z) = E_{\rho}\mathbf{e}_{r} + E_{\varphi}\mathbf{e}_{\varphi} + E_{z}\mathbf{e}_{z} = \begin{pmatrix} E_{\rho} \\ E_{\varphi} \\ E_{z} \end{pmatrix}$$
(4.27)

Therefore the TM modes can be written as

$$\mathbf{E}_{\bar{n}}^{\mathrm{TM}}(\mathbf{r}) = A^{\mathrm{TM}} \begin{pmatrix} 0 \\ 0 \\ R_m(\rho, k_{\bar{n}})\chi_m(\varphi) \end{pmatrix}.$$
(4.28)

We are considering TE modes of a homogeneous micro-cylinder so we can calculate the normalised $\mathbf{E}_{\bar{n}}$ from the $\mathbf{\bar{H}}_{\bar{n}}$ using the following simple relations derived in the Appendix D

$$\frac{n_r \nabla \times \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r})}{\varepsilon(\rho)k_n} = \mathbf{E}_{\bar{n}}(\mathbf{r})$$
(4.29)

which gives for $\rho \leq R$

$$\mathbf{E}_{\bar{n}}^{\mathrm{TE}}(\mathbf{r}) = \frac{n_r A^{\mathrm{TE}}(k_n)}{\varepsilon(\rho)k_n} \begin{pmatrix} \frac{R_m(\rho, k_{\bar{n}})}{\rho} \frac{d\chi_m(\varphi)}{d\varphi} \\ -\frac{\partial R_m(\rho, k_{\bar{n}})}{\partial\rho} \chi_m(\varphi) \\ 0 \end{pmatrix}$$
(4.30)

The LE modes are derived from the asymptotics of the Bessel function and the normalisation condition for longitudinal modes Eq. (2.29) for $\rho \leq R$,

$$\mathbf{E}_{n}^{\mathrm{LE}}(\mathbf{r}) = \sqrt{\left(\frac{2}{m(n_{r}^{2}+1)}\right)} \frac{\rho^{|m|-1}}{R^{|m|}} \begin{pmatrix} m\chi_{-m}(\varphi) \\ |m|\chi_{m}(\varphi) \\ 0 \end{pmatrix} (4.31)$$

4.1.3 The cut in the GF and its discretisation into cut poles

In this section we explain the origin of the cut in the GF and how it can in practice be discretised into a finite number of cut poles. The Hankel function $H_m(z)$ which describes the field outside the cylinder and contributes to Eq. (E.8) is a multiple-valued function, or in other words is defined on a Riemann surface having infinite number of sheets due to its logarithmic component. However, only one of these sheets contains the eigenvalues k_n , satisfying Eq. (4.23) or Eq. (4.24), which correspond to the outgoing wave boundary conditions of RSs. This 'physical' sheet of $H_m(z)$ has a cut in the complex z-plane along the negative imaginary half-axis, as we show in Appendix E, which in turn gives rise to the same cut in the GF. Consequently, the Mittag-Leffler theorem used for the spectral representation of the GF needs to be modified to include the cut contribution, as done in Appendix E.

For both the TM and TE case, treated here, the full GF of the homogeneous dielectric cylinder, which is defined via Maxwell's equation with a line current source term, is given by $\hat{\mathbf{G}}_k = G_k \, \mathbf{e}_z \otimes \mathbf{e}_z$, in which

$$G_k(\boldsymbol{\rho}, \boldsymbol{\rho}') = \sum_m G_m(\rho, \rho'; k) \chi_m(\varphi) \chi_m(\varphi'), \qquad (4.32)$$

and the radial components have the following spectral representation

$$G_{m}(\rho, \rho'; k) = \sum_{n} \frac{\left[A_{m}(k_{n})\right]^{2} R_{m}(\rho, k_{n}) R_{m}(\rho', k_{n})}{2k(k - k_{n})} + \int_{-i\infty}^{0} \frac{\left[A_{m}(k)\right]^{2} R_{m}(\rho, k') R_{m}(\rho', k')}{2k(k - k')} \sigma_{m}(k') dk' \equiv \sum_{n} \frac{\left[A_{m}(k_{n})\right]^{2} R_{m}(\rho, k_{n}) R_{m}(\rho', k_{n})}{2k(k - k_{n})}$$
(4.33)

derived in Appendix E. For TE modes we take $A_m(k) = A_m^{\text{TE}}(k)$ and for the TM modes we take $A_m(k) = A_m^{\text{TM}}$. The GF is for electric (magnetic) field in the TM (TE) case. Note that the cut contribution to the GF spectrum in the form of the integral in the last equation is described in terms of the *same functions* as those

used for discrete poles. This implies that the cut of the GF can be understood as a continuous distribution of additional poles along the negative imaginary half-axis with the density

$$\sigma_m(k) = \frac{8J_m(n_r kR)^2}{\pi^2 kR^2 D_m^+(kR) D_m^-(kR)} \frac{1}{A_m(k)^2}$$
(4.34)

calculated in Appendix E, with $D_m(kR)$ given by Eq. (4.25) in the case of the GF for TM modes or Eq. (4.26) in the case of the GF for the TE modes. Here $D_m^{\pm}(z)$ are the two limiting values of $D_m(z')$ for z' approaching point z on the cut from its different sides Re $z' \ge 0$. Remarkably, the integrated density of the cut contribution to the GF is equivalent to half a normal pole: $\int_{-i\infty}^0 \sigma_m(k) dk = (-1)^{m+1}/2$.



Figure 4.1: For the TM polarisation(a): Cut poles k_{α} (stars) representing the cut of the GF of a homogeneous dielectric cylinder with $n_r = 2$, in the complex wave-number plane for m = 0, 11, and 20. Normal poles k_n (open squares) are also shown. (b): Cut pole density $\sigma_m(k)$ (solid curves) and the cut pole strength $\phi_{\alpha}^{(m)}$ (stars), for the same values of m.

To numerically treat the cut contribution in the linear eigenvalue problem Eq. (2.35), one discretizes the integral in Eq. (4.33) into a finite number of cut poles

and adds cut RSs to the basis. These cut poles have non-integer strength $\phi_{\alpha}^{(m)}$ determined by the cut pole density σ_m . The function $\sigma_m(k)$ is purely imaginary and is peaked close to normal poles k_n as can be seen in Fig. 4.1 for selected m. In the numerical calculations we have used cut pole positions and strengths determined by splitting the cut interval $[0, -i\infty]$ into $N_c^{(m)}$ regions $[q_{\alpha}^{(m)}, q_{\alpha+1}^{(m)}]$ numbered by $\alpha = 1, 2, \ldots, N_c^{(m)}$, which are chosen to contain an equal weight according to

$$\int_{q_{\alpha}^{(m)}}^{q_{\alpha+1}^{(m)}} \sqrt{|\sigma_m(k)|} dk = \frac{1}{N_c^{(m)}} \int_{-i\infty}^0 \sqrt{|\sigma_m(k)|} dk.$$
(4.35)

For the numerical results shown later in this section and for the chosen values of $N_c^{(m)}$, using the weight $\sqrt{|\sigma_m|}$ in Eq. (4.35) was found to give the best accuracy of the RSE as compared to other powers of $|\sigma_m|$. Each region $[q_{\alpha}^{(m)}, q_{\alpha+1}^{(m)}]$ of the cut is represented by a cut pole of the GF at $k = k_{\alpha}^{(m)}$ given by the first moment,

$$k_{\alpha}^{(m)} = \int_{q_{\alpha}^{(m)}}^{q_{\alpha+1}^{(m)}} k\sigma_m(k) dk \middle/ \phi_{\alpha}^{(m)}, \qquad (4.36)$$

where the cut pole strength $\phi_{\alpha}^{(m)}$ is defined as

$$\phi_{\alpha}^{(m)} = \int_{q_{\alpha}^{(m)}}^{q_{\alpha+1}^{(m)}} \sigma_m(k) dk \,. \tag{4.37}$$

An example of cut poles for m = 0, 11, and 20 is given in Fig. 4.1(a) for the TM case (the TE case gives a similar result). The cut poles contribute to the RSE in the same way as the normal poles, and the matrix elements with the cut RSs are given by the overlap integrals Eq. (2.36) expressed in terms of exactly the same functions as for the normal RSs. In discretization of the linear eigenvalue problem of the RSE, the only modification caused by the cut is that the matrix of the perturbation is weighted according to the cut pole strengths $\phi_{\alpha}^{(m)}$ as shown in Eq. (4.4) and Eq. (4.5).

In the numerical calculation, the total number of poles N_t used in Eq. (2.35) determines the computational complexity of the matrix eigenvalue problem, so we are interested in the number of cut poles in the basis producing the best accuracy for a given N_t . We have investigated this numerically for the examples given below, and found that this is achieved using about 20% cut poles in the basis. Only for the homogeneous perturbation in Sec. 4.2.1, we used $N_c^{(m)} \sim N^{(m)}$, where $N^{(m)}$ is the number of normal poles in the basis for the given m, in order to demonstrate the convergence towards the exact solution. For all other numerical results we used $N_c^{(m)} \sim 0.2N^{(m)}$.

4.2 NUMERICAL RESULTS

In the following subsections we will give numerical results generated by the RSE for a range of perturbations to a homogeneous dielectric 2D microdisk in a vacuum, namely a homogeneous perturbation of the whole cylinder in Sec. 4.2.1, a half-cylinder perturbation in Sec. 4.2.2, a thin-film perturbation in Sec. 4.2.3 and a wire perturbation in Sec. 4.2.4. The basis system used will be a homogeneous dielectric cylinder of radius R and refractive index $n_r = 2$ ($\varepsilon = 4$). We will investigate how the convergence of the RSE depends on the dimensionality of the perturbation. In the case of thin wire perturbations Sec. 4.2.4 and homogeneous perturbation Sec. 4.2.1 we will show that the RSE is reproducing the results of the available analytic solutions. We give explicit forms of the matrix elements for these perturbations and details of their calculation in Appendix F.

4.2.1 Homogeneous Cylinder Perturbation

The perturbation we consider in this section is a homogeneous change of ε over the whole cylinder, given by

$$\Delta \varepsilon(\rho, \varphi) = \Delta \varepsilon \Theta(R - \rho) = \begin{cases} \Delta \varepsilon & \text{for } \rho \leq R, \\ 0 & \text{for } \rho > R \end{cases}$$
(4.38)

with the strength $\Delta \varepsilon = 4$ used in the numerical calculation. For φ -independent perturbations, modes with different azimuthal number m are decoupled, and so are even and odd (cosine and sine) modes given by Eq. (4.16). We show only the sine modes here, and use for illustration m = 20. We consider both TE and TM polarisations in this section. We calculate the matrix elements of the homogeneous perturbation analytically, the TM matrix elements are given by Eqs. (F.3)–(F.4) and the TE elements are given by Eqs. (F.5)– (F.9). The homogeneous perturbation does not change the geometry of the system, so that the perturbed modes obey the same secular equation Eqs. (4.23) and (4.24) with the refractive index n_r of the cylinder changed to $\sqrt{n_r^2 + \Delta \varepsilon}$, and thus the perturbed wave numbers \varkappa_{ν} calculated using the RSE can be compared with the exact values $\varkappa_{\nu}^{(\text{exact})}$.

We choose the basis of RSs for the RSE in such a way that for the given azimuthal number m and the given number of normal RSs N we find all normal poles $|k_n| < k_{\max}(N)$ with a suitably chosen maximum wave vector $k_{\max}(N)$ and then add the cut poles. We find that as we increase N, the relative error $|\varkappa_{\nu}/\varkappa_{\nu}^{(\text{exact})}-1|$ decreases as N^{-3} . Following the procedure described in Sec. 2.4 we can extrapolate the perturbed wave numbers. The resulting perturbed wave numbers are shown in Fig. 4.2 for the TM modes and Fig. 4.3 for the TE modes. The perturbation is strong, creating for TM and TE polarisation 3 additional WGMs with m = 20 having up to 4 orders of magnitude narrower linewidths. For N = 800, the RSE reproduces about 100 modes to a relative error in the 10^{-7} range, which is decreasing by one or two orders of magnitude after extrapolation. The contribution of the cut is significant: Ignoring the cut leads to a relative error of the poles in the 10^{-3} range. The fact that the relative error improves by 4-5 orders of magnitude after taking into account the cut in the form of the cut poles shows the validity of the reported analytical treatment of cuts in the RSE, and the high accuracy of the discretization method into cut poles. Missing out the LE mode results in several orders of magnitude higher relative error for the TE modes (see Fig. 4.3).



Figure 4.2: (a): Perturbed TM modes RS wave numbers for the homogeneous perturbation Eq. (5.17) calculated via the RSE with N = 800 (only sine modes are shown). The perturbed poles with (+) and without (×) the cut contribution are compared with the exact solution (open squares). Unperturbed wave numbers are also shown (open circles with dots). Inset: Dielectric constant profile for the unperturbed and perturbed systems. (b): Relative error in the calculated perturbed wave numbers with (heptagons) and without (triangles) contribution of the cut. Relative error for a simulation including the cut and improved by extrapolation is also shown (crossed circles).



Figure 4.3: (a): Perturbed TE modes RS wave numbers for the homogeneous perturbation Eq. (5.17) calculated via the RSE with N = 800 (only sine modes are shown). The perturbed poles with (+) and without (×) the cut contribution are compared with the exact solution (open squares). Unperturbed wave numbers are also shown (open circles with dots). Inset: Dielectric constant profile for the unperturbed and perturbed systems. (b): Relative error in the calculated perturbed wave numbers with (heptagons) and without (triangles) contribution of the cut and LE mode. Relative error for a simulation including the cut and improved by extrapolation is also shown (crossed circles).

4.2.2 Half-Cylinder Perturbation

We now consider a bulk perturbation which mixes modes with different m. The perturbation is given by

$$\Delta \varepsilon(\rho, \varphi) = \Delta \epsilon \Theta(R - \rho) (1 - 2\Theta(\pi/2 - |\varphi|))$$
(4.39)

In our numerical simulation we take $\Delta \epsilon = 0.2$. The matrix elements of the perturbation are given by Eqs. (F.11)–(F.13) which require a numerical integration. Owing to the symmetry of the perturbation, the sine and cosine basis modes are still decoupled, therefore we treat them separately, see panels (a) and (b) in Fig. 4.4. Due to a relatively small perturbation (compared to that considered in Sec. 4.2.1), the mode positions in the spectrum do not change much. However, the quality factors Q of all WGMs decrease, as the lifetime of the resonances is now limited by an additional scattering at the step in the dielectric constant of the perturbed cylinder. Due to isotropy TE and TM modes are decoupled allowing us to treat only TM modes in this subsection.

To the best of our knowledge, an analytic solution for this perturbation is not available and thus we cannot calculate the relative error of the RSE result with respect to the exact solution. However, we can investigate the convergence of the method in order to demonstrate how the RSE works in this case, which is not reducible to an effective one-dimensional problem. We do this in Fig. 4.4 showing the perturbed sine and cosine modes for two different values of basis size N and in Fig. 4.5 where absolute errors M_{ν} are shown for several different values of N. Following Sec. 2.4, the absolute error is defined here as $M_{\nu} = \max_{i=1,2,3} |\varkappa_{\nu}^{N_4} - \varkappa_{\nu}^{N_i}|$, where $\varkappa_{\nu}^{N_i}$ are the RS wave numbers calculated for basis sizes of $N_1 \approx N/2$, $N_2 \approx N/\sqrt{2}$, $N_3 \approx N/\sqrt[4]{2}$, and $N_4 = N$. The results for the cosine and sine modes are quite similar. From Fig. 5.4 we see that the perturbed resonances are converging with increasing basis size.

We were able to see the power law of the convergency, in agreement with Sec. 3.2. We found that the power law exponent is approximately -2. We found however that owing to the above mentioned fluctuations, the power law convergence is not well developed compared to the one-dimensional problems considered so far



Figure 4.4: Unperturbed (open circles with dots) and perturbed RS wave numbers of (a) cosine and (b) TM sine modes of a cylinder for a half-cylinder perturbation Eq. (4.39) with $\Delta \varepsilon = 0.2$ and the basis sizes N = 2000 (crosses) and N = 4000 (hexagons). Only the WGM region is shown. Inset: Diagram showing the regions of increased (solid blue) and decreased (red striped) dielectric constant.



Figure 4.5: Absolute errors M_{ν} of the RS wave numbers \varkappa_{ν} for the TM modes subjected to the half-cylinder perturbation Eq. (4.39) as functions of Re \varkappa_{ν} , calculated via the RSE for different basis sizes N, for cosine (closed shapes) and sine (open shapes) modes.

(including the example of Sec. 4.2.1). Increasing the basis size N improves the powerlaw convergency. This is attributed to the larger number of basis states below a given $|k_{\max}R|$ in effective 2D systems compared to effective 1D systems. Thus one needs a larger basis in order to approximate discrete steps of the basis size by a continuous power law.

To show how one of the perturbed states is created as superposition of unperturbed states, we show by a star in Fig. 4.6 one the perturbed WGMs of Fig. 4.4 (a) as a superposition which, owing to the perturbation, increases its linewidth by nearly an order of magnitude. The contribution of the basis states is visualized by circles of a radius proportional to $|c_{n\nu}|^{1/3}$, which are centered at the positions of the wave vectors k_n in the complex k-plane. The expansion coefficients $c_{n\nu}$ decrease quickly with the distance to the spectral position of the perturbed mode \varkappa_{ν} , with the dominant contribution coming from the nearest unperturbed RS, a typical feature of perturbation theory in closed systems. Importantly, this demonstrates that if we are interested in the modes within a small spectral region, one can limit the basis in the RSE to states close to that region. This result is crucial for the application of the RSE to effective 3D systems which have even larger numbers of basis states below a given $|k_{\max}R|$, as one can significantly reduce the number of basis states needed to calculate the perturbation of a mode of interest to a given accuracy.



Figure 4.6: Contributions of the basis RSs (black circles) to a given perturbed RS (blue star), calculated for the cosine TM modes and the half-cylinder perturbation Eq. (4.39), using N = 4000. All circles and the star are centered at the positions of the corresponding RS wave numbers in the complex k-plane. The radius of the circles are proportional to $|c_{n\nu}|^{1/3}$. A key showing the relationship between circle radius and $|c_{n\nu}|^2$ is given by the dark blue circles.

4.2.3 Thin-Film Perturbation

Here we consider the case of a thin film embedded in the cylinder, corresponding to a line perturbation in the effective 2D system. The perturbation we consider in this section is given by

$$\Delta \varepsilon(\rho, \varphi) = h \Delta \varepsilon \, \frac{\Theta(R - \rho)}{\rho} \, \delta(\varphi) \,, \tag{4.40}$$

see the inset in Fig. 4.8. In our numerical simulation we take the strength of the perturbation $h\Delta\varepsilon = -0.1R$. Physically this perturbation corresponds to a thin metal film of uniform negative dielectric constant $n_r^2 + \Delta\epsilon$ and width h much narrower than the shortest wavelength in the basis. The perturbation leaves the sine modes of the unperturbed cylinder unchanged. Hence we only include cosine modes into the basis. The perturbation matrix elements are given by Eq. (F.14). Due to isotropy TE and TM modes are decoupled allowing us to treat only TM modes in this subsection.

To our knowledge an analytic solution for this perturbation is not known and we therefore calculate the absolute error as in Sec. 4.2.2. Fig. 4.8 shows the resulting RS wave numbers and absolute errors for this thin-film perturbation. We see in Fig. 4.8(b) that the convergence of the RSE is slower than in the case of the halfmoon perturbation. This is expected as the thin film has no geometrical effect on the wave-vector k_y , giving higher contributions of basis states with large k_y , similar to the results in 1D with a delta scatterer perturbation reported earlier Sec. 3.2.4. We have found that the power law exponent in this case is approximately -1.

4.2.4 Thin-Wire Perturbation

As the last example of the chapter we consider a dielectric cylinder perturbed by a thin-wire perturbation which is represented by small disk of radius b centered at the point **d** on the x-axis ($\varphi = 0$). We do not use here a delta perturbation, in order to compare it with an analytic solution available in the literature [41]. The perturbation is defined as

$$\Delta \varepsilon(\boldsymbol{\rho}) = \Delta \varepsilon \Theta(b - |\boldsymbol{\rho} - \mathbf{d}|), \qquad (4.41)$$

and we choose $d = |\mathbf{d}| = 0.8R$, b = 0.001R, and $\Delta \epsilon = 100$ (the unperturbed system is the same as before having $n_r = 2.0$). This perturbation leaves the sine and cosine



Figure 4.7: (a): Unperturbed and perturbed RS wave numbers of TM cosine modes for a thin-film perturbation given by Eq. (4.40) with $h\Delta\varepsilon = -0.1R$, calculated via the RSE with the basis sizes N = 2000 (crosses) and N = 4000 (hexagons). The unperturbed RSs are shown as open circles with dots. (b): Absolute errors M_{ν} as functions of Re \varkappa_{ν} calculated for different basis sizes N as labeled. Inset: Sketch showing the location of the thin metal film perturbation as a red line inside the unperturbed cylinder.

modes decoupled, and the sine modes approximately unchanged (strictly for $d \to 0$). Therefore we show here the perturbation of the cosine modes. Due to isotropy TE and TM modes are decoupled allowing us to treat only TM modes in this subsection. The RSE perturbation matrix elements are given by Eq. (F.16). The resulting RS wave numbers are shown in Fig. 4.8 (a) together with the analytic approximation derived in Ref.[41], demonstrating a good agreement. The absolute errors M_{ν} are shown in Fig. 4.8 (b). We see that the convergence in the case of a thin wire is even slower than for the thin-film perturbation shown in Sec. 4.2.3. This is expected as the thin wire has no geometrical effect on both k_x and k_y , giving higher contributions of the basis states with large |k|. We found that within the basis sizes investigated, the power law is not well developed, but for weaker (smaller $|\Delta \epsilon|$) or more spatially extended (larger b) perturbations a better convergence is observed, as expected.

The analytic solution of Ref.[41] for a point-like scatterer in a 2D disk is not strict in any physical system. In the case of a delta scatterer, the secular equation is logarithmically divergent and thus cannot be used, while the accuracy of the model for a finite size scatterer relies on a number of approximations [40, 41] which require $|n_r \varkappa_{\nu} b| \ll 1$, $|\varkappa_{\nu} b \sqrt{n_r^2 + \Delta \epsilon}| \ll 1$, and also $|\text{Re} \varkappa_{\nu}| \gg |\text{Im} \varkappa_{\nu}|$, i.e. having a large Q. In addition to this, the point-like perturbation should not be too close to the edge of the disk, i.e. $|n_r \varkappa_{\nu} (R - d)| \ll 1$. While we have chosen the parameters to be suitable for these approximations, we do not have a quantitative estimate of the error. Nevertheless, the comparison in Fig. 4.8 (a) of the RSE calculation with the analytic solution demonstrates a good agreement which is improving as we move closer to the origin in the complex k-plane, as detailed in Fig. 5.6 (b) where the absolute difference between the two calculations is shown.

4.3 SUMMARY

We have applied the RSE to effective two-dimensional (2D) open optical systems with $k_z = 0$, such as dielectric micro-cylinders and micro-disks with perturbations. We have found and treated a cut of the GFs of effective 2D systems – a feature which to our knowledge has not been mentioned in the literature but turned out to



Figure 4.8: (a): Unperturbed and perturbed RS wave numbers of TM cosine modes for a thin-wire perturbation given by Eq. (4.41) with d = 0.8R, b = 0.001R, and $\Delta \varepsilon = 100$, calculated via the RSE with the basis size N = 2000 (crosses) and compared with the analytic approximation of Ref.[41] (empty squares). The unperturbed basis states are shown as open circles with dots. (b): Absolute errors M_{ν} in RSE as functions of Re \varkappa_{ν} calculated for different basis size N and the absolute difference between the RSE and the analytic approximation (crosses \times). Inset: Sketch showing the location of the wire as a red dot inside the unperturbed cylinder.

be crucial for the RSE as the states on the cut contribute to the completeness of the basis of RSs needed for the accuracy of the method. We have detailed the formulation of the RSE for a general 2D case treating all polarisations and shown how the theory is applied to effective 2D systems for which states on the cut are introduced and discretized for the numerics.

Using the analytically known basis of resonant states (RSs) of an ideal homogeneous dielectric cylinder – a complete set of eigenmodes satisfying outgoing wave boundary conditions – we have treated different types of perturbations, such as halfcylinder, thin-film and thin-wire perturbations. For all of these perturbations, the perturbed systems are not reducible to effective 1D ones, so that the present work demonstrates the applicability of the RSE to general effective 2D perturbations which mix all basis modes. We investigated the convergency for these perturbations and compared the RSE results, where it was possible, with available analytic solutions. In particular, we have made such a comparison for a homogeneous perturbation of a cylinder, which is reducible to an effective 1D system, and for point-like perturbation of a disk which presents an essentially 2D system with mixing of all kind of modes in the given polarization of light. In both situations we have found agreement between the RSE and the known analytic solutions.

Chapter 5

RSE applied to three-dimensional open optical systems

In this chapter we extend the resonant state expansion formulation to arbitrary threedimensional (3D) open optical systems, compare its performance with FDTD and FEM, and introduce a local perturbation approach. The chapter is organized as follows. In Sec. 5.1 we treat the homogeneous dielectric sphere as the unperturbed system and the resulting basis for the RSE consisting of normalized transverse electric (TE) and transverse magnetic (TM) modes, as well as longitudinal zero frequency modes. This is followed in Sec. 5.2 by examples illustrating the method and comparing results with existing analytic solutions, as well as numerical solutions provided by using available commercial software. We demonstrate the performance of RSE as a local perturbation method for selected modes by introducing a procedure to select a suited subset of basis states.

5.1 EIGENMODES OF A DIELECTRIC SPHERE AS BASIS FOR THE RSE

To apply the RSE to 3D systems we need a known basis of RSs. We choose here the RSs of a dielectric sphere of radius R and refractive index n_r , surrounded by vacuum, since they are analytically known. For any spherically symmetric system, the solutions of Maxwell's equations split into four groups: TE, TM, and longitudinal electric (LE) and longitudinal magnetic (LM) modes [48]. TE (TM) modes have no radial components of the electric (magnetic) field, respectively. Longitudinal modes were introduced in Sec. 4.1.3. Owing to the spherical symmetry, the azimuthal quantum number m and total angular momentum quantum number l are eigenvalues of the angular momentum operator and take integer values corresponding to the number of field oscillations around the sphere. For each l value there are 2l + 1 degenerate modes with m = -l..l.

Following Ref.[48], the three groups of modes of a homogeneous dielectric sphere can be written as

TE:
$$\mathbf{E} = -\mathbf{r} \times \nabla f$$
 and $i\mathbf{H} = \frac{\nabla \times \mathbf{E}}{k}$,
TM: $i\mathbf{H} = -\mathbf{r} \times \nabla f$ and $\mathbf{E} = \frac{\nabla \times i\mathbf{H}}{\varepsilon k}$, (5.1)
LM: $\mathbf{H} = -\nabla f$ and $\mathbf{E} = 0$,
LE: $\mathbf{E} = -\nabla f$ and $\mathbf{H} = 0$,

where $f(\mathbf{r})$ is a scalar function satisfying the Helmholtz equation

$$\nabla^2 f + k^2 \varepsilon f = 0, \qquad (5.2)$$

with the permittivity of the dielectric sphere in vacuum given by

$$\varepsilon(r) = \begin{cases} n_r^2 & \text{for } r \leq R \\ 1 & \text{for } r > R. \end{cases}$$
(5.3)

Owing to the spherical symmetry of the system, the solution of Eq. (5.2) splits in spherical coordinates $\mathbf{r} = (r, \theta, \varphi)$ into the radial and angular components:

$$f(\mathbf{r}) = R_l(r,k)Y_{lm}(\Omega), \qquad (5.4)$$

where $\Omega = (\theta, \varphi)$ with the angle ranges $0 \leq \theta \leq \pi$ and $-\pi \leq \varphi \leq \pi$. The angular

component is given by the spherical harmonics,

$$Y_{lm}(\Omega) = \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta)\chi_m(\varphi), \qquad (5.5)$$

which are the eigenfunctions of the angular part of the Laplacian,

$$\hat{\Lambda}(\Omega)Y_{lm}(\Omega) = -l(l+1)Y_{lm}(\Omega), \qquad (5.6)$$

where $P_l^m(x)$ are the associated Legendre polynomials. The azimuthal functions are defined by Eq. (4.16). The radial components $R_l(r,k)$ satisfy the spherical Bessel equation,

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \varepsilon(r)k^2\right]R_l(r,k) = 0$$
(5.7)

and have the following form

$$R_l(r,k) = \begin{cases} j_l(n_rkr)/j_l(n_rkR) & \text{for } r \leq R\\ h_l(kr)/h_l(kR) & \text{for } r > R \end{cases}$$
(5.8)

in which $j_l(z)$ and $h_l(z) \equiv h_l^{(1)}(z)$ are, respectively, the spherical Bessel and Hankel functions of the first kind.

In spherical coordinates, a vector field $\mathbf{E}(\mathbf{r})$ can be written as

$$\mathbf{E}(r,\theta,\varphi) = E_r \mathbf{e}_r + E_{\theta} \mathbf{e}_{\theta} + E_{\varphi} \mathbf{e}_{\varphi} = \begin{pmatrix} E_r \\ E_{\theta} \\ E_{\varphi} \end{pmatrix},$$

where \mathbf{e}_r , \mathbf{e}_{θ} , and \mathbf{e}_{φ} are the unit vectors. The electric field of the RSs then has the form

$$\mathbf{E}_{n}^{\mathrm{TE}}(\mathbf{r}) = A_{l}^{\mathrm{TE}} R_{l}(r, k_{n}) \begin{pmatrix} 0 \\ \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} Y_{lm}(\Omega) \\ -\frac{\partial}{\partial \theta} Y_{lm}(\Omega) \end{pmatrix}$$
(5.9)

for TE modes,

$$\mathbf{E}_{n}^{\mathrm{TM}}(\mathbf{r}) = \frac{A_{l}^{\mathrm{TM}}(k_{n})}{\varepsilon(r)k_{n}r} \begin{pmatrix} l(l+1)R_{l}(r,k_{n})Y_{lm}(\Omega) \\ \frac{\partial}{\partial r}rR_{l}(r,k_{n})\frac{\partial}{\partial \theta}Y_{lm}(\Omega) \\ \frac{\partial}{\partial r}\frac{rR_{l}(r,k_{n})}{\sin\theta}\frac{\partial}{\partial \varphi}Y_{lm}(\Omega) \end{pmatrix}$$
(5.10)

for TM modes, and

$$\mathbf{E}_{n}^{\mathrm{LE}}(\mathbf{r}) = A_{l}^{\mathrm{LE}} \begin{pmatrix} \frac{\partial}{\partial r} R_{l}(r,0) Y_{lm}(\Omega) \\ \frac{R_{l}(r,0)}{r} \frac{\partial}{\partial \theta} Y_{lm}(\Omega) \\ \frac{R_{l}(r,0)}{r \sin \theta} \frac{\partial}{\partial \varphi} Y_{lm}(\Omega) \end{pmatrix}$$
(5.11)

for LE modes. They are normalized according to Eqs. (2.23)-(2.29), leading to the following normalization constants:

$$A_{l}^{\text{TE}} = \sqrt{\frac{2}{l(l+1)R^{3}(n_{r}^{2}-1)}},$$

$$\frac{n_{r}A_{l}^{\text{TE}}}{A_{l}^{\text{TM}}(k)} = \sqrt{\left[\frac{j_{l-1}(n_{r}kR)}{j_{l}(n_{r}kR)} - \frac{l}{n_{r}kR}\right]^{2} + \frac{l(l+1)}{k^{2}R^{2}}},$$

$$A_{l}^{\text{LE}} = \sqrt{\frac{2}{R(n_{r}^{2}l+l+1)}}.$$
(5.12)

Longitudinal magnetic modes have zero electric field, and since we limit ourselves in this work to perturbations in the dielectric susceptibility only, they are not mixed by the perturbation to other types of modes and are thus ignored in the following.

The Maxwell boundary conditions following from Eq. (4.11), namely the continuity of the tangential components of **E** and **H** across the spherical dielectric-vacuum interface, lead to the following secular equations determining the RS wavenumbers k_n :

$$\frac{n_r j_l'(n_r z)}{j_l(n_r z)} - \frac{h_l'(z)}{h_l(z)} = 0$$
(5.13)

for TE modes and

$$\frac{n_r j_l'(n_r z)}{j_l(n_r z)} - \frac{n_r^2 h_l'(z)}{h_l(z)} - \frac{n_r^2 - 1}{z} = 0$$
(5.14)

for TM modes, where $z = k_n R$ and $j'_l(z)$ and $h'_l(z)$ are the derivatives of $j_l(z)$ and $h_l(z)$, respectively. While the LE modes are the RSs easiest to calculate due to a simple power-law form of their radial functions,

$$R_{l}(r,0) = \begin{cases} (r/R)^{l} & \text{for } r \leq R \\ (R/r)^{l+1} & \text{for } r > R \end{cases}$$
(5.15)

it is convenient to treat them in the RSE as part of the TM family of RSs. Indeed, for $r \leq R$ they coincide with the TM modes taken in the limit $k_n \to 0$:

$$\mathbf{E}_{n}^{\text{LE}}(\mathbf{r}) = \sqrt{l(n_{r}^{2}-1)} \lim_{k_{n} \to 0} \mathbf{E}_{n}^{\text{TM}}(\mathbf{r}) \,.$$
(5.16)

Note that $k_n = 0$ is not a solution of the secular equation (5.14) for TM modes. However, using the analytic dependence of the wave functions of TM modes on k_n [see Eqs. (5.8), (5.10), and (5.12)], the limit in Eq. (5.16) can be taken in the calculation of the matrix elements containing LE modes. The same limit $k_n \to 0$ has to be approached in the matrix eigenvalue problem Eq. (2.35) of the RSE, as the matrix elements are divergent, due to the $1/\sqrt{k_n}$ factor introduced in the expansion coefficients. It is found that adding a finite negative imaginary part to static poles, $k_n R = -i\delta$, with δ typically of order 10^{-7} (determined by the numerical accuracy) is suited for the numerical results presented in the following section. We have verified this by comparing the results with the ones of the RSE in the form of a generalized linear eigenvalue problem Eq. (2.34), which has no such divergence, but its numerical solution is a factor of 2-3 slower in the NAG library implementation.

5.2 NUMERICAL RESULTS FOR 3D SYSTEMS WITH SCALAR DIELECTRIC SUSCEPTIBILITY

In this section we discuss the application of the RSE to 3D systems described by a scalar dielectric function $\hat{\boldsymbol{\varepsilon}}(\mathbf{r}) + \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) = \hat{\mathbf{1}}[\boldsymbol{\varepsilon}(r) + \Delta \boldsymbol{\varepsilon}(\mathbf{r})]$. As the unperturbed system we use the homogeneous dielectric sphere of radius R with $\boldsymbol{\varepsilon}(r)$ given by Eq. (5.3), having the analytical modes discussed in Sec. 5.1. We use the refractive index $n_r = 2$ of the unperturbed sphere throughout this section and consider several types of perturbations, namely, a homogeneous perturbation of the whole sphere in Sec. 5.2.1, a half-sphere perturbation in Sec. 5.2.2, and a quarter-sphere perturbation in Sec. 5.2.3. We demonstrate in Sec. 5.3 the performance of the RSE as a local perturbation method for a chosen group of modes by introducing a way to select a suitable subset of basis states. Explicit forms of the matrix elements used in these calculations are given in Appendix G.

5.2.1 Homogeneous sphere perturbation

The perturbation we consider here is a homogeneous change of ε over the whole sphere, given by

$$\Delta \varepsilon(\mathbf{r}) = \Delta \epsilon \Theta(R - r) \,, \tag{5.17}$$

where Θ is the Heaviside function, with the strength $\Delta \epsilon = 5$ used in the numerical calculation. For spherically symmetric perturbations, RSs of different angular quantum numbers (l, m), and different transverse polarizations are not mixed, and are degenerate in m. We show here for illustration the l = 5 modes. The matrix elements of the perturbation Eq. (5.17) are given by Eqs.(G.1)–(G.5) of Appendix G. The homogeneous perturbation does not change the structure of the system, so that the perturbed modes obey the same secular equations Eq. (5.13) and Eq. (5.14) with the refractive index n_r of the sphere changed to $\sqrt{n_r^2 + \Delta \epsilon}$, and the perturbed wavenumbers \varkappa_{ν} calculated using the RSE can be compared with the exact values $\varkappa_{\nu}^{(\text{exact})}$ obtained from the secular equations.

We choose the basis of RSs for the RSE in such a way that for a given orbital



Figure 5.1: TM RSs with l = 5 (and a fixed m) for the homogeneous perturbation Eq. (5.17) with $\Delta \epsilon = 5$. (a) perturbed RSs wavenumbers calculated using RSE with N = 1000 with (+) and without (×) the LE mode, as well as using the exact secular equation (open squares). The wavenumbers of the unperturbed system are shown as open circles with dots. Inset: Dielectric constant profile of the unperturbed (black line) and perturbed (red line) systems. (b) Relative error of the perturbed wavenumbers calculated with (+) and without (×) contribution of the LE mode, as well as with the LE mode and extrapolation (crossed heptagons).



Figure 5.2: As Fig. 5.1 but for TE RSs, for which the LE modes have no influence.

number l and m we select all RSs with $|k_n| < k_{\max}(N)$ using a maximum wave vector $k_{\max}(N)$ chosen to result in N RSs. We find that as we increase N, the relative error $|\varkappa_{\nu}/\varkappa_{\nu}^{(\text{exact})} - 1|$ decreases as N^{-3} . Following the procedure described Sec. 2.4 we extrapolate the perturbed wavenumbers. The resulting perturbed wavenumbers for N = 1000 (corresponding to $k_{\max}R = 400$) are shown in Fig. 5.1 for the TM RSs and Fig. 5.2 for the TE RSs. The perturbation is strong, leading to WGMs with up to 2 orders of magnitude narrower linewidths. The RSE reproduces the wavenumbers of about 100 RSs to a relative error in the 10^{-7} range, which is improved further by one to two orders of magnitude after extrapolation. The homogeneous perturbation does not couple LE modes to TE modes as LE modes have the symmetry of TM modes
[see Eq. (5.16)] leading to vanishing overlap integrals with TE RSs. The contribution of the LE-mode RS in the TM polarization is significant, as is shown in Fig. 5.1 by the large decrease of the relative error by up to 8 orders of magnitude when adding them to the basis. This validates the analytical treatment of the LE-mode RSs in the RSE developed in this work. We have verified that taking a finite imaginary value of $\delta = 10^{-7}$ in Eq. (2.35) for the LE-modes instead of using strict $k_n = 0$ poles in Eq. (2.34), as done throughout this work, changes the relative error of the TM mode calculation by less than 10% and within the range of 10^{-9} only. For practical applications, this limitation should not be relevant as the error in the measured geometry will typically be significantly larger.

5.2.2 Hemisphere Perturbation

We consider here a hemisphere perturbation as sketched in Fig. 5.3 which mixes TE, TM, and LE modes with different l, while conserving m. The perturbation is given by

$$\Delta \varepsilon(\mathbf{r}) = \Delta \epsilon \Theta(R - r) \Theta\left(\theta - \frac{\pi}{2}\right)$$
(5.18)

and increases ε in the northern hemisphere by $\Delta \epsilon$, while leaving the southern hemisphere unchanged. In our numerical simulation, we use $\Delta \epsilon = 0.2$. The calculation of the matrix elements is done using Eqs. (G.7)–(G.12) of Appendix G which require numerical integration. Owing to the symmetry of the perturbation, matrix elements between TM and TE RSs can only be non-zero when the RSs have m of opposite sign and equal magnitude, i.e. they are are sine and cosine states of equal |m|. Similarly, matrix elements between two TE RSs or two TM RSs can only be non-zero if both states have the same m. We can therefore restrict the basis to m = 3 TM states and m = -3 TE states for the numerical calculations of this section. We treat the LE RSs as TM modes with $k_n R = -i10^{-7}$ and a normalization factor modified according to Eq. (5.16). The resulting RS wavenumbers are shown in Fig. 5.3. Due to the smaller perturbation compared to that considered in Sec. 5.2.1, the mode positions in the spectrum do not change as much. The imaginary part of most of the WGMs decreases due to the higher dielectric constant in the perturbed hemisphere. However,



Figure 5.3: (a) Unperturbed and perturbed RS wavenumbers for a hemisphere perturbation given by Eq. (5.18) with $\Delta \epsilon = 0.2$, for |m| = 3, calculated via the RSE with basis sizes of N = 2000 (crosses) and N = 4000 (hexagons). The unperturbed RSs are shown as open circles with dots. (b) Absolute errors M_{ν} as function of Re \varkappa_{ν} calculated for different basis sizes N as labeled. Inset: Diagram illustrating a dielectric sphere with the regions of increased (lower hemisphere) and decreased (upper hemisphere) dielectric constant.

some of the modes also have an increased imaginary part due to the scattering at the edge of the perturbation.

To the best of our knowledge, an analytic solution for this perturbation is not available and thus we cannot calculate the relative error of the RSE result with respect to the exact solution. However, we can investigate the convergence of the method in order to demonstrate how the RSE works in this case, for the perturbation not reducible to an effective one-dimensional problem. We accordingly show in Fig. 5.3(a) the perturbed modes for two different values of basis size N and in Fig. 5.3(b) the absolute errors M_{ν} for several different values of N. Following the procedure of Sec. 2.4, the absolute error is defined here as $M_{\nu} = \max_{i=1,2,3} |\varkappa_{\nu}^{N_4} - \varkappa_{\nu}^{N_i}|$, where $\varkappa_{\nu}^{N_i}$ are the RS wavenumbers calculated for basis sizes of $N_1 \approx N/2$, $N_2 \approx N/\sqrt{2}$, $N_3 \approx N/\sqrt{2}$, and $N_4 = N$. We see that the perturbed resonances are converging with increasing basis size, approximately following a power law with an exponent between -2 and -3.

5.2.3 Quarter-Sphere Perturbation and comparison with FEM/FDTD methods

We consider here a perturbation which breaks both continuous rotation symmetries of the sphere and is thus is not reducible to an effective one or two-dimensional system. The perturbation is given by

$$\Delta \varepsilon(\mathbf{r}) = \Delta \epsilon \Theta(R - r) \Theta\left(\frac{\pi}{2} - \theta\right) \Theta\left(|\varphi| - \frac{\pi}{2}\right)$$
(5.19)

and corresponds physically to a uniform increase of the dielectric constant in a quarter-sphere area, as sketched in Fig. 5.4. In our numerical simulation, we take $\Delta \epsilon = 1$. Again, the calculation of the matrix elements requires numerical integration. Owing to the reduced symmetry of the perturbation as compared to that treated in the previous section we now have modes of different l, m, and polarization mixing, although TE sine (TM cosine) and TE cosine (TM sine) modes are decoupled, owing to the mirror symmetry of the system. This allowed me to split the simulation of



Figure 5.4: (a) Unperturbed and perturbed RS wavenumbers for a quarter-sphere perturbation given by Eq. (5.19) with $\Delta \epsilon = 1$, calculated by the RSE with the basis sizes N = 4000 (crosses) and N = 8000 (hexagons). The unperturbed RSs are shown as open circles with dots. A sketch of the perturbation geometry is also shown. (b) Zoom of (a) showing the splitting of a 2l + 1 degenerate WGMs as the *m* degeneracy is lifted. Here l = 7. The pole indicated in (b) by an arrow is analyzed further in Fig. 5.6. The results of FEM simulations using 200k, 100k, 50k and 25k finite elements are shown for comparison. (c) Absolute error M_{ν} as function of Re \varkappa_{ν} calculated by the RSE with different basis sizes N as labeled, for the RSs shown in (b).

all modes into two separate simulations called A and B, respectively, each of size N. Simulation A (B) correspond to TE sin mode and TM cos modes (TM sin mode and TE cos modes). The lifting of the *m*-degeneracy of the unperturbed modes can be seen as splitting off resonances in Fig. 5.4(a) and (b). In most cases the splitting in the real part of the resonant wavenumber is greater than the linewidth of the modes.

The convergence of the RSE is well seen in Fig. 5.4(a) and (b) showing the perturbed RS wavenumbers for two different basis sizes N. An analytic solution for this perturbation is not available, so we use the method described in Sec. 2.4 to estimate the error, and show in Fig. 5.4(c) the resulting absolute errors M_{ν} for several values of N. A convergence with a power law exponent between -2 and -3 is again observed, resulting in relative errors in the 10^{-4} to 10^{-5} range for N = 8000.

To verify the RSE results, we have simulated the system using the commercial solver ComSol (http://www.comsol.com) which uses the finite element method and Galerkin's method, approximating the openness of the system with an absorbing perfectly matched layer (PML). We have surrounded the sphere with a vacuum shell followed by a PML shell of equal thickness D. The results are shown in Fig. 5.4(b) using D = R/2, and a "physics controlled" mesh with $N_{\rm G} = 25$ k, 50k, 100k and 200k finite elements. We used the nearest unperturbed RS wave vector as the linearization point (i.e. the input value) for the ComSol solver, and requested the determination of 40 eigenfrequencies, which we found to be the minimum number reliably returning all 15 non-degenerate modes deriving from the l = 7 unperturbed fundamental WGM. With increasing $N_{\rm G}$, the ComSol RS wavenumbers tend towards the RSE poles, with an error scaling approximately as $N_{\rm G}^{-1}$. This is verifying the validity of the RSE results.

To make a comparison between the RSE and ComSol in terms of numerical complexity we use the poles computed by an N = 16000 RSE simulation as the "exact solution" to calculate the average relative errors of the poles shown in Fig. 5.4(b) versus effective processing time on an Intel E8500 CPU. The result is shown in Fig. 5.5, including ComSol data for different shell thicknesses D of R/2, R/4, and R/8, revealing that D = R/4 provides the best performance. This comparison shows that the RSE is 2-3 orders of magnitude faster than ComSol for the present example, and at



Figure 5.5: A comparison of the relative error of the perturbed RS wavenumbers shown in Fig. 5.4(b) calculated by the RSE for different N as labeled versus computational time. For comparison, the performance of the FEM using ComSol, and FDTD using Lumerical are given. In the FEM we have used a thickness of the vacuum layer and the perfectly matched layer of R/2, R/4, and R/8 as labeled, and $N_{\rm G}=25$ k, 50k, 100k, 200k finite elements as labeled. In the FDTD we used different grid spacings from R/8to R/80 and other parameters as given in the text.

the same time determines significantly more RSs.

The RSE computing time includes the calculation of the matrix elements which were done evaluating the 1-dimensional integrals (see Appendix G.2) using 10000 equidistant grid points. The computing time of the matrix elements is significant only for $N \leq 2000$, while for larger N the matrix diagonalization time, scaling as N^3 , is dominating. We have verified that the accuracy of the matrix element calculation is sufficient to not influence the relative errors shown.

We also include in Fig. 5.5 the performance of FDTD calculations using the commercial software Lumerical (http://www.lumerical.com) [49]. They were undertaken using a simulation cube size from 2.5R to 4R, exploiting the reflection symmetry, and for grid steps between R/8 and R/80, with a sub-sampling of 32. The simulation area was surrounded by a PML of a size chosen automatically by the software. The excitation pulse had a centre wavenumber of kR = 5.1 and a relative bandwidth of 10% to excite the relevant modes, and the simulation was run for 360 oscillation periods. The calculated time-dependent electric field after the excitation pulse was transformed into a spectrum and the peaks were fitted with a Lorentzian to determine the real and imaginary part of the mode. The parameters used were chosen to optimize the performance, and in the plot the results with the shortest computation time for a given relative error are given.

We can conclude that the RSE is about two orders of magnitude faster than both FEM and FDTD for this specific problem, showing its potential to supersede presently used methods. A general analysis of the performance of RSE relative to FEM and FDTD will be the subject of our future research.

To illustrate how a particular perturbed RS is created as a superposition of unperturbed RSs, we show in Fig. 5.6 the contributions of the unperturbed RSs to the perturbed WGM indicated by the arrow in Fig. 5.4(b) with index ν and wavenumber \varkappa_{ν} , given by the open star in Fig. 5.6. The contribution of the basis states to this mode are visualized by circles of a radius proportional to $\sqrt[6]{\sum |c_{n\nu}|^2}$, where the sum is taken over the 2l+1 degenerate basis RSs of a given eigenfrequency, centered at the positions of the RS wavenumbers in the complex k-plane. The expansion coefficients $c_{n\nu}$ decrease quickly with the distance between the unperturbed and perturbed RS wavenumbers, with the dominant contribution coming from the nearest unperturbed RS, a typical feature of perturbation theory in closed systems. The unperturbed RS nearest to the perturbed one in Fig. 5.6 has the largest contribution, and is a l = 7TE WGM with the lowest radial quantum number. Other WGMs giving significant contributions have the same radial quantum number and the angular quantum numbers ranging between l = 6 and l = 9, see the small stars in Fig. 5.6 corresponding to l = 7 basis states. This is a manifestation of a quasi-conservation of the angular momentum l for bulk perturbations like the quarter-sphere perturbation considered here.

Generally, we see that a significant number of unperturbed RSs are contributing to the perturbed RS, which is indicating that previous perturbation theories for



Figure 5.6: (a) Contributions of the basis RSs (blue and red circles) to the perturbed RS (open star) indicated by an arrow in Fig. 5.5(b), calculated using the RSE with N = 8000. Small stars show the positions of l = 7 TE modes. All circles and stars are centred at the positions of the corresponding RS wavenumbers in the complex k-plane. The radius of the circles is proportional to $\sqrt[6]{\sum |c_{n\nu}|^2}$, where the sum is taken over all *m*-degenerate RSs of the basis system corresponding to the given eigenfrequency. A key showing the relationship between circle radius and $\sum |c_{n\nu}|^2$ is given as black circles. (b) A zoom of (a) showing the contribution of RSs close to the chosen perturbed state. The angular quantum numbers l of the WGMs with the largest contributions are indicated.

open systems would yield large errors for the strong perturbations treated in this work since they are limited to low orders [50, 51] or to degenerate modes only [52].

5.3 LOCAL PERTURBATION

The weights of the RSs shown in Fig. 5.6 indicate that a perturbed mode can be approximately described by a subset of the unperturbed modes, which typically have wavenumbers in close proximity to that of the perturbed mode. It is therefore expected that a local perturbation approach based on the RSE is possible. We develop such an approach.

We commence with a small subset S of modes of the unperturbed system which are of particular interest, for example because they are used for sensing. To calculate the perturbation of these modes approximately, we consider a global basis \mathcal{B} as used in the previous sections, with a size N providing a sufficiently small relative error. We then choose a subset $S^+ \subset \mathcal{B}$ with N' < N elements containing S, i.e. $S \subset S^+$, and solve the RSE Eq. (2.35) restricted to S^+ . The important step in this approach is to find a numerically efficient method to choose the additional modes in S^+ which provide the smallest relative error of the perturbed states deriving from Sfor a given N'. Specifically, the method should be significantly faster than the matrix diagonalization Eq. (2.35).

To develop such a method, we consider here the Rayleigh-Schrödinger perturbation theory based on the RSE and expand the RS wave vector \varkappa up to second order,

$$\frac{1}{\varkappa} = \left(\frac{1}{\varkappa}\right)^{(0)} + \left(\frac{1}{\varkappa}\right)^{(1)} + \left(\frac{1}{\varkappa}\right)^{(2)} + \dots, \qquad (5.20)$$

where

$$\left(\frac{1}{\varkappa}\right)^{(0)} = \frac{1}{k_n}, \quad \left(\frac{1}{\varkappa}\right)^{(1)} = \frac{V_{nn}}{2k_n}, \quad \left(\frac{1}{\varkappa}\right)^{(2)} = -\frac{1}{4}\sum_{n'\neq n}\frac{V_{nn'}^2}{k_n - k_{n'}} \tag{5.21}$$

as directly follows from Eq. (2.35). Note that the second-order result in Eq. (5.21) is different from that given in Ref. [50].

We can expect that the second-order correction given by Eq. (5.21) is a suited candidate to estimate the importance of modes. We therefore sort the modes in \mathcal{B} according to the weight W_n given by

$$W_n = \sum_{n' \in \mathcal{D}} \sum_{n'' \in \mathcal{S}} \left| \frac{V_{n'n''}^2}{k_{n'} - k_{n''}} \right|,$$
(5.22)

where \mathcal{D} is the set of modes degenerate with the mode n in \mathcal{B} . The summation over all degenerate modes is motivated by their comparable contribution to the perturbed mode, as known from degenerate perturbation theory. We add modes of \mathcal{B} to \mathcal{S}^+ in decreasing W_n order. Groups of degenerate modes \mathcal{D} are added in one step as they have equal W_n . A special case are the LE modes in the basis of the dielectric sphere, which are all degenerate having $k_n = 0$. They are added in groups of equal l in the order of reducing weight.

To exemplify the local perturbation method, we use the quarter sphere perturbation with two different perturbations strengths $\Delta \epsilon = 1$ and $\Delta \epsilon = 0.2$, and choose the degenerate l = 7 modes shown in Fig. 5.4(b) as S. The perturbed RSs deriving from S are shown in Fig. 5.7(a) and (b), as calculated by RSE using either a global basis \mathcal{B} with N = 16000, or a minimum local basis $S^+ = S$ with $N' \sim 10$, or a larger S^+ with $N' \sim 100$. As in the previous section we show the results separately for each class of RSs (A and B) decoupled by symmetry. We see that for $\Delta \epsilon = 0.2$ ($\Delta \epsilon = 1$) the perturbation lifts the degeneracy of S by a relative wavenumber change of about 1% (5%), and that the minimum local basis $S^+ = S$ of only degenerate modes reproduces the wavenumbers with a relative error of about 10^{-4} (10^{-3}), i.e. the perturbation effect is reproduced with an error of a few %. Increasing the local basis size to $N' \sim 100$ the error reduces by a factor of three, by similar absolute amounts in the real and the imaginary part of the wavenumber [see insets of Fig. 5.7(a) and (b)].

The relative error of the local-basis RSE is generally decreasing with increasing basis size, as shown in Fig. 5.7(c). It can however be non-monotonous on the scale of individual sets of degenerate modes. This is clearly seen for for $\Delta \epsilon = 0.2$ and small N', where adding the second group increases the error, which is reverted when the third group is added. These groups are the l = 6 and l = 8 fundamental WGMs as expected from Fig. 5.6(b), which are on opposite sides of S (l = 7 WGMs) in the complex frequency plane. Adding only one of them therefore imbalances the result,



Figure 5.7: (a) Unperturbed and perturbed RS wavenumbers for a quarter-sphere perturbation given by Eq. (5.19) with $\Delta \epsilon = 1$, calculated by the RSE using the local basis sizes N' = 7, 8 (+), N' = 99, 103 (×) for the parts A,B, respectively, and a global basis with N = 16000 (hexagons). The unperturbed RSs are shown as a circle with a dot. The inset is a zoom to the RS with the strongest perturbation. (b) As in (a) but for $\Delta \epsilon = 0.2$. (c) Average relative error of the states shown in (a) and (b) versus basis size for a global basis (squares and crosses), and for a local basis (circles) derived from a global basis of N = 8000 modes.

leading to an increase of the relative error.

Comparing results in Fig. 5.7(c) for two different values of $\Delta \epsilon$, we see that the second-order correction dominates the relative error, as in the wide range of N' the error scales approximately like a square of the perturbation strength. The global-basis RSE, also shown in Fig. 5.7(b), has for a given basis size significantly larger errors. Furthermore, a minimum basis size is required for the basis to actually contain S, in the present case $N \approx 500$. The local basis thus provides a method to calculate the perturbation of arbitrary modes with a small basis size.

The local perturbation method described in this section enables the calculation of high frequency perturbed modes which have previously been numerically inaccessible to FDTD and FEM due to the necessity of the corresponding high number of elements needed to resolve the short wavelengths involved and inaccessible to the RSE with a global basis due to the prohibitively large N required. The example we used for the illustration shows that a basis of ~ 100 RSs in the local RSE can be sufficient to achieve the same accuracy as provided by FDTD and FEM in a reasonable computational time [see Figs. 5.5 and 5.7(c)]. For this basis size, solving the RSE Eq. (2.35) is 6 orders of magnitude faster than FDTD and FEM, and the computational time in our numerical implementation is dominated by the matrix element calculation which can be further optimized. A detailed evaluation of the performance of the local basis RSE and a comparison of selection criteria different from Eq. (5.22) will be the subject of our future research.

5.4 SUMMARY

We have applied the resonant state expansion (RSE) to general three-dimensional (3D) open optical systems. This required including in the basis both types of transversal polarization states, TE and TM modes, as well as longitudinal electric field modes at zero frequency. Using the analytically known basis of resonant states (RSs) of a dielectric sphere – a complete set of eigenmodes satisfying outgoing wave boundary conditions – we have applied the RSE to perturbations of full-, half- and quarter-sphere shapes. The latter does not have any rotational or translational symmetry

and is thus not reducible to lower dimensions, so that their treatment demonstrates the applicability of the RSE to general 3D perturbations.

We have compared the performance of the RSE with commercially available solvers, using both the FEM and FDTD, and showed that for the geometries considered here, the RSE is several orders of magnitude more computationally efficient, showing its potential to supersede presently used computational methods in electrodynamics. We have furthermore introduced a local perturbation method for the RSE, which is restricting the basis in order to treat a small subset of modes of interest. This further reduces computational efforts and improves on previous local perturbation methods.

Chapter 6

Conclusion

We have further developed the RSE, a new method for calculating the GF of open systems by expressing it as a spectrum of RSs. The RSs provide a natural discretisation of a GF. This representation of the GF makes it possible to formulate an equation relating perturbed RSs to the perturbation and the unperturbed GF. We have used this equation in the derivation of the matrix equation which can be solved to give the perturbed RSs as an expansion of the unperturbed RSs. For homogeneous planar, cylindrical, and spherical systems the RSs can be calculated analytically. Since these unperturbed RSs are analytic, using them in the RSE can make the calculation of the RSs for a perturbed system more efficient than FDTD or FEM methods which are fully numerical.

I will now summarise the theoretical developments in detail that we have presented in this thesis.

6.1 General formulation of RSE for open systems

Previous applications of the RSE were limited to systems described by scalar equations so the key theoretical developments of this thesis are mathematical derivations and proofs which have allowed the RSE to become a mathematically rigorous perturbation theory for two and three-dimensional systems. As part of the general formulation of the RSE we develop algorithms for measuring and extrapolating this convergence to the exact solution.

6.2 Application to planar systems

Chapter 3 details the application of the RSE to planar open optical systems such as layered dielectric slabs and Bragg reflector microcavities. It is demonstrated that the RSE converges with a power law in the basis size. Algorithms for error estimation and their reduction are evaluated. We calculate relative errors for the results of RSE by comparison with scattering matrix methods for the fields and also transcendental equations in the case of eigenfrequencies.

The planar system is then examined further by considering non-normal incidences of light and numerical evaluation of the convergence of RSE to exact analytic results is made. Interestingly, the spectral analysis of a dielectric slab in terms of resonant states reveals an influence of waveguide modes in the transmission. These modes, which on resonance do not couple to external light, surprisingly do couple to external light for off-resonant excitation.

6.3 Application to two and three-dimensional systems

In chapter 4 we detail the application of the RSE to 2-dimensional open optical systems considering all possible polarisations but limited to zero in-line momentum. We use the homogeneous dielectric cylinder as the basis system. We use GF theory to show that the RSE basis requires the inclusion of a continuum of resonant states with imaginary eigenfrequency. This continuum is discretised and included in the basis. The complex eigenfrequencies are calculated for a selection of perturbations which are effectively 2-dimensional such as half-cylinder, thin-film, and thin wire. We show the RSE reproduces the eigenfrequencies of an approximative analytic solution in the case of the thin-wire perturbation. In Chapter 5 we apply the RSE to three-dimensional open optical systems. The analytically solvable homogeneous dielectric sphere is used as the basis system. Since any perturbation which is breaking the spherical symmetry is mixing TE and TM modes the RSE is extended to use TM modes and the zero frequency pole of the GF. We investigate the convergence of the RSE for perturbations which sequentially reduce the number of continuous symmetries of our systems from 2 to 1 to zero . We find that the RSE provides a higher accuracy than the FEM and FDTD for a given computational effort, demonstrating its potential to replace presently used methods.

6.4 LOCAL PERTURBATION METHOD

At the end of chapter 5 we develop a local perturbation method for RSE, which is a unique capability of the RSE as compared to FEM or FDTD. The local perturbation method makes it in principle practical to use the RSE to calculate weakly perturbed high frequency modes using just the modes that are contributing strongly to the perturbed modes of interest. Therefore the local perturbation method in this section could allow the calculation of high frequency perturbed modes which have previously been numerically inaccessible by FDTD and FEM due to the necessity of the corresponding high number of elements needed to resolve the short wavelengths involved and previously not accessible to the RSE due to the prohibitively large basis required by that method.

6.5 FUTURE WORK

Our future RSE research might be a theoretical extension of the method to treat photonic crystal fibre optic cables with non zero in-line momentum for the purposes of optimising their loss, dispersion, and bandwidth, important for sensing and communications technologies. We could then extend the investigations of [53] by designing the optimum fibres with the RSE as a fast and economical alternative to experimental studies. The RSE also has potential for commercialization, as its performance can supersede FEM and FDTD because its efficiency can be orders of magnitude better. The commercialization of RSE as a new solver for electrodynamic problems will impact a wide range of additional fields, including also quantum optics, photonic circuits, photonic materials and nano plasmonics.

Appendix A

Mittag-Leffler theorem applied to electrodynamic GF

The residue theorem in mathematics states

Let γ be a contour, and let f be a function holomorphic in an open domain \mathcal{U} containing $I(\gamma) \cup \gamma^*$, except for finitely many poles $c_1, c_2, ..., c_m$ in $I(\gamma)$ then

$$\int_{\gamma} f(z)dz = 2\pi i \sum_{k=1}^{m} \operatorname{Res}(f, c_k)$$
(A.1)

where $\operatorname{Res}(f, c_k)$ is the residue of f at c_k .

If we take \mathcal{U} to be an open set in the complex plane, then in mathematics a function f(z) is said to be holomorphic in \mathcal{U} if it is differentiable at every point in \mathcal{U} .

The definition of differentiability for a complex function at a point c is there must exist

$$\lim_{z \to c} \frac{f(z) - f(c)}{z - c} = f'(c)$$
(A.2)

where f'(c) is the derivative of f at c. f'(c) must be the same if we approach c from all possible directions.

We find in this thesis that not all the GFs to which we apply the residue theorem meet this condition on every subspace of the complex frequency plane. We find the non-differentiable regions are cuts or lines of discontinuity in the GF. We find that γ must be deformed to avoid these regions. We can use the residue theorem to derive the Mittag-Leffer theorem we let

$$f(k') = \frac{\hat{\mathbf{G}}_{k'}(\mathbf{r}, \mathbf{r}')}{k' - k}$$
(A.3)

then the residue theorem implies

$$\int_{\gamma} \frac{\hat{\mathbf{G}}_{k'}(\mathbf{r}, \mathbf{r}')}{k' - k} dk' = 2\pi i \hat{\mathbf{G}}_{k}(\mathbf{r}, \mathbf{r}') + 2\pi i \sum_{n} \frac{\operatorname{Res}(\hat{\mathbf{G}}_{k''}(\mathbf{r}, \mathbf{r}'), k_{n})}{k - k_{n}}.$$
 (A.4)

Thus the Mittag-Leffer theorem allows us to write $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}')$ as a function of a contour integral and its poles or resonances. In our case $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}')$ is the GF satisfying the electrodynamic GF Eq. (2.2) with outgoing BCs.

In most cases the asymptotic $G_k(z, z') \propto k^{-2}$ for $|k| \to \infty$ allow us to approximate the path integral in Eq. (A.4) as zero [30, 32].

Appendix B

Spectral representation of the GFs of an open system

The Green's function (GF) of an open electromagnetic system is a tensor $\hat{\mathbf{G}}_k$ which satisfies the outgoing wave BCs and the Maxwell wave equation Eq. (2.1) with a delta function source term,

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}'), \qquad (B.1)$$

where $\hat{\mathbf{1}}$ is the unit tensor. Physically, the GF describes the response of the system to a point current with frequency ω , i.e. an oscillating dipole.

We assuming a simple-pole structure of the GF with poles at $k = q_n$ and take into account its large-k vanishing asymptotics. Therefore the Mittag-Leffler theorem[30, 32] (see Appendix A) allows us to express the GF as

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\hat{\mathbf{Q}}_{n}(\mathbf{r},\mathbf{r}')}{k-q_{n}}.$$
(B.2)

We assume no degeneracy for the mode n. The definition of the residue $\hat{\mathbf{Q}}_n(\mathbf{r}, \mathbf{r}')$ at a simple pole of the function $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}')$ is,

$$\lim_{k \to q_n} (k - q_n) \hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}') = \hat{\mathbf{Q}}_n(\mathbf{r}, \mathbf{r}'), \qquad (B.3)$$

where we have again assumed $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}')$ to be holomorphic in this neighbourhood of k_n except for at the poles k_n so that it has a Laurent series at k_n . Substituting the expression Eq. (B.2) into Eq. (B.3) gives

$$\lim_{k \to q_n} (k - q_n) \sum_m \frac{\hat{\mathbf{Q}}_m(\mathbf{r}, \mathbf{r}')}{k - q_m} = \hat{\mathbf{Q}}_n(\mathbf{r}, \mathbf{r}')$$
(B.4)

so that

$$\lim_{k \to q_n} (k - q_n) \sum_{m \neq n} \frac{\hat{\mathbf{Q}}_m(\mathbf{r}, \mathbf{r}')}{k - q_m} = 0$$
(B.5)

Substituting the expression Eq. (B.2) into Eq. (B.1) and convoluting with an arbitrary finite field $\mathbf{D}(\mathbf{r})$ over a finite volume V we obtain

$$\sum_{n} \frac{-\nabla \times \nabla \times \mathbf{F}_{n}(\mathbf{r}) + k^{2} \varepsilon(\mathbf{r}) \mathbf{F}_{n}(\mathbf{r})}{k - q_{n}} = \mathbf{D}(\mathbf{r}), \qquad (B.6)$$

where $\mathbf{F}_n(\mathbf{r}) = \int_V \hat{\mathbf{Q}}_n(\mathbf{r}, \mathbf{r}') \mathbf{D}(\mathbf{r}') d\mathbf{r}'$. Multiplying by $(k - q_n)$ and taking the limit $k \to q_n$ yields

$$\lim_{k \to q_n} (k - q_n) \sum_n \frac{-\nabla \times \nabla \times \mathbf{F}_n(\mathbf{r}) + k^2 \varepsilon(\mathbf{r}) \mathbf{F}_n(\mathbf{r})}{k - q_n} = \lim_{k \to q_n} (k - q_n) \mathbf{D}(\mathbf{r}) = 0.$$
(B.7)

From Eq. (B.5) we can see,

$$\lim_{k \to q_n} (k - q_n) \sum_{m \neq n} \frac{-\nabla \times \nabla \times \mathbf{F}_m(\mathbf{r}) + k^2 \varepsilon(\mathbf{r}) \mathbf{F}_m(\mathbf{r})}{k - q_m} = 0, \qquad (B.8)$$

so we can drop terms $n \neq m$ from the summation in Eq. (B.7) to give

$$\lim_{k \to q_n} (k - q_n) \frac{-\nabla \times \nabla \times \mathbf{F}_n(\mathbf{r}) + k^2 \varepsilon(\mathbf{r}) \mathbf{F}_n(\mathbf{r})}{k - q_n} = 0.$$
(B.9)

or

$$-\nabla \times \nabla \times \mathbf{F}_n(\mathbf{r}) + q_n^2 \varepsilon(\mathbf{r}) \mathbf{F}_n(\mathbf{r}) = 0.$$
 (B.10)

Due to the convolution with the GF, $\mathbf{F}_n(\mathbf{r})$ satisfies the same outgoing wave BCs Eq. (2.7). Then, according to Eq. (2.6), $\mathbf{F}_n(\mathbf{r}) \propto \mathbf{E}_n(\mathbf{r})$ and $q_n = k_n$. Note that the convolution of the kernel $\hat{\mathbf{Q}}_n(\mathbf{r}, \mathbf{r}')$ with different functions $\mathbf{D}(\mathbf{r})$ can be proportional to one and the same function $\mathbf{E}_n(\mathbf{r})$ only if the kernel has the form of a direct product:

$$\hat{\mathbf{Q}}_n(\mathbf{r},\mathbf{r}') = \mathbf{E}_n(\mathbf{r}) \otimes \mathbf{E}_n(\mathbf{r}') / w_n , \qquad (B.11)$$

with $w_n = 2k_n$, a normalisation factor. The symmetry in Eq. (B.11) follows from the reciprocity theorem [54], described mathematically by the relation

$$\mathbf{d}_1 \hat{\mathbf{G}}_k(\mathbf{r}_1, \mathbf{r}_2) \mathbf{d}_2 = \mathbf{d}_2 \hat{\mathbf{G}}_k(\mathbf{r}_2, \mathbf{r}_1) \mathbf{d}_1, \qquad (B.12)$$

which holds for any two dipoles $\mathbf{d}_{1,2}$ at points $\mathbf{r}_{1,2}$ oscillating with the same frequency. Hence $\hat{\mathbf{G}}_k(\mathbf{r}, \mathbf{r}')$ is a symmetric tensor.

In the case of a Green's function made up of degenerate modes we modify the proof of Eq. (B.11) by making use of orthogonality of the degenerate modes to choose $\mathbf{D}(\mathbf{r})$ such that,

$$\int_{V} \mathbf{E}_{m}(\mathbf{r}) \cdot \mathbf{D}(\mathbf{r}) \, d\mathbf{r} = 0 \,, \tag{B.13}$$

for $m \neq n$ and where state m is degenerate with n.

Appendix C

Analytic RSs and perturbation matrices for planar open optical systems

C.1 RSs of a slab perturbed by a wide dielectric layer in the case of normal incidence

The exact solutions of the wave equation Eq. (3.3) with p = 0 for the system with the perturbation given by Eq. (3.13) and outgoing boundary conditions have the form

$$\mathcal{E}_{\nu}^{(\text{exact})}(z) = \begin{cases} A_{\nu}e^{-i\varkappa_{\nu}z}, & z < -a, \\ B_{\nu}e^{i\sqrt{\epsilon_{s}}\varkappa_{\nu}z} + C_{\nu}e^{-i\sqrt{\epsilon_{s}}\varkappa_{\nu}z}, & -a \leq z \leq b, \\ D_{\nu}e^{i\sqrt{\epsilon_{p}}\varkappa_{\nu}z} + E_{\nu}e^{-i\sqrt{\epsilon_{p}}\varkappa_{\nu}z}, & b \leq z \leq a, \\ H_{\nu}e^{i\varkappa_{\nu}z}, & z > a, \end{cases}$$
(C.1)

where $\epsilon_p = \epsilon_s + \Delta \epsilon$, and b = a/2. We find the coefficients in Eq. (C.1) from the continuity of the electric field and its derivative and the normalization condition Eq. (3.15). The complex-valued RS wave numbers \varkappa_{ν} are found by solving a secular equation following from the boundary conditions:

$$\beta \gamma f(k)g(k) - 1 = \frac{\beta - \gamma}{\beta \gamma - 1} \Big[\beta g(k) - \gamma f(k) \Big], \qquad (C.2)$$

where

$$\beta = \frac{\sqrt{\epsilon_p} + 1}{\sqrt{\epsilon_p} - 1},\tag{C.3}$$

$$\gamma = \frac{\sqrt{\epsilon_s} + 1}{\sqrt{\epsilon_s} - 1},\tag{C.4}$$

and the functions f(k) and g(k) are defined as

$$f(k) = e^{-2i\sqrt{\epsilon_s}k(a+b)}, \quad g(k) = e^{-2i\sqrt{\epsilon_s}k(a-b)}.$$
 (C.5)

We solve Eq. (C.2) using the Newton-Raphson method to find $k = \varkappa_{\nu}^{\text{(exact)}}$.

C.2 MATRIX ELEMENTS OF THE WIDE-LAYER PERTUR-BATION FOR ARBITRARY IN-PLANE WAVEVECTOR P

Using Eq. (2.36) or Eq. (2.49) and basis functions Eq. (3.5) we calculate V_{nm} for the wide-layer perturbation Eq. (3.13) to be

$$V_{nm} = \Delta \epsilon B_n B_m \Big[\eta(q_n + q_m, z) + (-1)^m \eta(q_n - q_m, z) \\ + (-1)^n \eta(q_m - q_n, z) + (-1)^{n+m} \eta(-q_n - q_m, z) \Big]_b^a,$$

for $n \neq m$ and

$$V_{nn} = \Delta \epsilon B_n^2 \Big[2(-1)^n z + \eta(2q_n, z) + \eta(-2q_n, z) \Big]_b^a$$
(C.6)

for n = m, where $\eta(k, z) = e^{i\sqrt{\epsilon_s}kz}/ik$.

C.3 RSs of a slab perturbed by a δ perturbation for p=0

In the case of a δ -perturbation $\Delta \varepsilon(z) = w \epsilon_d \delta(z-b)$ with $|b| \leq a$ and p = 0, we find the secular equation for the RS wave vectors takes the form

$$\left[1 + \gamma f(k)\right] \left[1 + \gamma g(k)\right] = \frac{2i\sqrt{\epsilon_s}}{w\epsilon_d k} \left[1 - \gamma^2 f(k)g(k)\right].$$
(C.7)

where f and g are the functions derived above. Eq. (C.7) is also solved numerically with the help of the Newton-Raphson method to find $k = \varkappa_{\nu}^{(\text{exact})}$.

C.4 Matrix elements of the δ -perturbation

Using Eq. (3.12) and basis functions Eq. (3.5) we calculate V_{nm} for the δ perturbation to be

$$V_{nm} = w\epsilon_d E_n(a/2)E_m(a/2).$$
(C.8)

Appendix D

Normalised transverse electric modes of a cylinder expressed in terms of normalised magnetic modes

The Green's function for the magnetic component of an electrodynamic system is a tensor $\hat{\mathbf{G}}_k^{\mathrm{H}}$ which satisfies the outgoing wave boundary conditions and Maxwell's wave equation with a delta function source term

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times (\nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')) + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')$$
$$= \hat{\mathbf{1}} \delta(\mathbf{r} - \mathbf{r}') . \quad (\mathrm{D.1})$$

following the derivation for the spectral representation of $\hat{\mathbf{G}}_k$ in Sec. 4.1.1 we find $\hat{\mathbf{G}}_k^{\mathrm{H}}$ can be written as

$$\hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\beta_{\bar{n}} \phi_{\bar{n}} \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}) \otimes \bar{\mathbf{H}}_{\bar{n}}(\mathbf{r}')}{2k_{n}(k-k_{\bar{n}})}.$$
 (D.2)

If we only consider the region inside of the optical resonator Eq. (2.2) become

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') + k^{2} \varepsilon \hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}')$$
(D.3)

where

$$\hat{\mathbf{G}}_{k}(\mathbf{r},\mathbf{r}') = \sum_{n} \frac{\alpha_{\bar{n}} \phi_{\bar{n}} \mathbf{E}_{\bar{n}}(\mathbf{r}) \otimes \mathbf{E}_{\bar{n}}(\mathbf{r}')}{2k(k-k_{\bar{n}})}.$$
 (D.4)

Again if we only consider the region inside of the optical resonator Eq. (D.1) become

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') + k^{2} \varepsilon \hat{\mathbf{G}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') = \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}')$$
(D.5)

We have introduced the normalisation factors $\alpha_{\bar{n}}$ and $\beta_{\bar{n}}$.

We now consider two functions \mathbf{F} and \mathbf{J} which are zero outside of the optical resonator and on the border. Convoluting Eq. (D.3) with \mathbf{F} and Eq. (D.5) with \mathbf{J} we obtain,

$$-\nabla \times \nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r},\mathbf{r}') + k^{2} \varepsilon \hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r},\mathbf{r}') = \mathbf{F}(\mathbf{r})$$
(D.6)

$$-\nabla \times \nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') + k^{2}\varepsilon \hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}') = \mathbf{J}(\mathbf{r})$$
(D.7)

We calculate $\hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r},\mathbf{r}')$ from the spectral Green's function Eq. (D.4) to be

$$\hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r}) = \sum_{n} \frac{\alpha_{n} \mathbf{E}_{n}(\mathbf{r}) f_{n}}{2k_{n}(k - k_{n})} \tag{D.8}$$

We calculate $\hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r},\mathbf{r}')$ from the spectral Green's function Eq. (D.2) to be

$$\hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r}) = \sum_{n} \frac{\beta_{n} \bar{\mathbf{H}}_{n}(\mathbf{r}) g_{n}}{2k_{n}(k - k_{n})} \tag{D.9}$$

The constant f_n is calculated to be

$$f_n = \int_V \mathbf{E}_n(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r}) d\mathbf{r}$$
(D.10)

The constant g_n is calculated to be

$$g_n = \int_V \bar{\mathbf{H}}_n(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r}) d\mathbf{r}$$
(D.11)

We define V to be the volume where $\mathbf{J}(\mathbf{r}) \neq 0$ and $\mathbf{F}(\mathbf{r}) \neq 0$.

We can see by comparing Eq. (2.1) and Eq. (4.7) that $\mathbf{J}(\mathbf{r})$ is proportional to

 $\nabla \times \mathbf{F}(\mathbf{r})$ because $\mathbf{J}(\mathbf{r})$ plays the role of the oscillating current in both equations. Hence without lose of generality we may let $\mathbf{J}(\mathbf{r}) = \nabla \times \mathbf{F}(\mathbf{r})$ and use Maxwell's equations,

$$\nabla \times \mathbf{E}_n(\mathbf{r}) = ik_n \bar{\mathbf{H}}_n(\mathbf{r}) \tag{D.12}$$

$$\nabla \times \bar{\mathbf{H}}_n(\mathbf{r}) = -ik_n \varepsilon \mathbf{E}_n(\mathbf{r}) \tag{D.13}$$

we find

$$\nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{E}}(br) = i \sum_{n} \frac{\alpha_{n} \mathbf{H}_{n}(\mathbf{r}) f_{n}}{2(k-k_{n})}$$
(D.14)

Taking the curl of Eq. (D.6) gives,

$$-\nabla \times (\nabla \times \nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r},\mathbf{r}')) + k^{2}\varepsilon(\nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r},\mathbf{r}')) = \nabla \times \mathbf{F}(\mathbf{r})$$
(D.15)

We can rewrite g_n in terms of f_n

$$g_n = \int_V \bar{\mathbf{H}}_n(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r}) d\mathbf{r} = \int_V \bar{\mathbf{H}}_n(\mathbf{r}) \cdot \nabla \times \mathbf{F}(\mathbf{r}) d\mathbf{r}$$
$$= \int_S \bar{\mathbf{H}}_n(\mathbf{r}) \times \mathbf{F}(\mathbf{r}) dS + \int_V \mathbf{F}(\mathbf{r}) \cdot \nabla \times \bar{\mathbf{H}}_n(\mathbf{r}) d\mathbf{r}. \quad (D.16)$$

However $\mathbf{F}(\mathbf{r}) = 0$ on the surface S, therefore

$$g_n = -ik_n \varepsilon \int_V \mathbf{E}_n(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r}) d\mathbf{r} = -ik_n \varepsilon f_n \tag{D.17}$$

Then we see Eq. (D.9) can be written,

$$\hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r}) = \sum_{n} \frac{-i\beta_{n}\bar{\mathbf{H}}_{n}(\mathbf{r})\varepsilon f_{n}}{2(k-k_{n})}$$
(D.18)

Compare Eq. (D.15) and Eq. (D.7) we obtain $\nabla \times \hat{\mathbf{P}}_{k}^{\mathrm{E}}(\mathbf{r}) = \hat{\mathbf{P}}_{k}^{\mathrm{H}}(\mathbf{r})$, then equating coefficients at the pole k_{n} we find,

$$-\beta_n \varepsilon = \alpha_n \tag{D.19}$$

Appendix E

Green's function of a homogeneous cylinder

The TM component of the GF $\hat{\mathbf{G}}_{k}^{\text{TM}}(\mathbf{r}, \mathbf{r}')$ for the electric field in the case of a homogeneous cylinder in vacuum satisfies the following equation

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{TM}}(\mathbf{r},\mathbf{r}') + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}^{\mathrm{TM}}(\mathbf{r},\mathbf{r}') = \hat{\mathbf{1}} \delta(\mathbf{r}-\mathbf{r}'), \qquad (E.1)$$

The TE component of the GF $\hat{\mathbf{G}}_{k}^{\text{TE}}(\mathbf{r}, \mathbf{r}')$ for the magnetic field in the case of a homogeneous cylinder in vacuum satisfies the following equation

$$-\nabla \times \nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{TE}}(\mathbf{r},\mathbf{r}') + \hat{\boldsymbol{\varepsilon}}(\mathbf{r})^{-1} \nabla \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \times (\nabla \times \hat{\mathbf{G}}_{k}^{\mathrm{TE}}(\mathbf{r},\mathbf{r}')) + k^{2} \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \hat{\mathbf{G}}_{k}^{\mathrm{TE}}(\mathbf{r},\mathbf{r}')$$
$$= \hat{\mathbf{1}} \delta(\mathbf{r} - \mathbf{r}'), \quad (E.2)$$

where $\mathbf{r}=(\rho,\varphi,z)$ and

$$\varepsilon(\mathbf{r}) = \begin{cases} n_r^2 & \text{for } \rho \leq R, \\ 1 & \text{for } \rho > R. \end{cases}$$
(E.3)

Using the angular basis Eq. (4.16) both TM and TE GFs can be written as

$$G_k(\boldsymbol{\rho}, \boldsymbol{\rho}') = \frac{1}{\sqrt{\rho\rho'}} \sum_m \tilde{G}_m(\rho, \rho'; k) \chi_m(\varphi) \chi_m(\varphi'), \qquad (E.4)$$

similar to Eq. (4.32). Note that we redefined here the radial part as $\tilde{G}_m(\rho, \rho'; k) = \sqrt{\rho \rho'} G_m(\rho, \rho'; k)$ which satisfies in the TM case

$$\left[\frac{d^2}{d\rho^2} - \frac{m^2 - 1/4}{\rho^2} + k^2 \varepsilon(\rho)\right] \tilde{G}_m^{\text{TM}}(\rho, \rho'; k) = \delta(\rho - \rho').$$
(E.5)

or in the TM case for magnetic field,

$$\begin{bmatrix} \frac{d^2}{d\rho^2} - \frac{m^2 - 1/4}{\rho^2} + \frac{1}{\varepsilon(\rho)} \frac{d\varepsilon(\rho)}{d\rho} \frac{1}{2\rho} \end{bmatrix} \tilde{G}_m^{\text{TE}}(\rho, \rho'; k) + \\ + \left[k^2 \varepsilon(\rho) - \frac{1}{\varepsilon(\rho)} \frac{d\varepsilon(\rho)}{d\rho} \frac{d}{d\rho} \right] \tilde{G}_m^{\text{TE}}(\rho, \rho'; k) = \delta(\rho - \rho') \,.$$
(E.6)

Using two linearly independent solutions $f_m(\rho)$ and $g_m(\rho)$ of the corresponding homogeneous equation which satisfy the asymptotic boundary conditions

$$f_m(\rho) \propto \rho^{m+1/2} \quad \text{for} \quad \rho \to 0 \,,$$

$$g_m(\rho) \propto e^{ik\rho} \quad \text{for} \quad \rho \to \infty \,.$$

the GF can be expressed as

$$\tilde{G}_m(\rho, \rho'; k) = \frac{f_m(\rho_<)g_m(\rho_>)}{W(f_m, g_m)},$$
(E.7)

in which $\rho_{<} = \min\{\rho, \rho'\}, \rho_{>} = \max\{\rho, \rho'\}$, and the Wronskian W(f, g) = fg' - f'g. For TM polarization, a suitable pair of solutions is given by

$$f_m(\rho) = \sqrt{\rho} \cdot \begin{cases} J_m(n_r\rho k), & \rho \leq R, \\ a_m J_m(\rho k) + b_m H_m(\rho k), & \rho > R, \end{cases}$$
$$g_m(\rho) = \sqrt{\rho} \cdot \begin{cases} c_m J_m(n_r\rho k) + a_m H_m(n_r\rho k), & \rho \leq R, \\ H_m(\rho k), & \rho > R, \end{cases}$$

where for TM modes

$$\begin{aligned} a_m^{\rm TM}(k) &= \left[n_r J'_m(n_r x) H_m(x) - J_m(n_r x) H'_m(x) \right] \pi i x/2 \,, \\ b_m^{\rm TM}(k) &= \left[J'_m(x) J_m(n_r x) - n_r J_m(x) J'_m(n_r x) \right] \pi i x/2 \,, \\ c_m^{TM}(k) &= \left[H'_m(x) H_m(n_r x) - n_r H_m(x) H'_m(n_r x) \right] \pi i x/2 \end{aligned}$$

or for TE modes

$$a_m^{\text{TE}}(k) = [H_m(x)J'_m(n_r x) - n_r H'_m(x)J_m(n_r x)]\pi ix/2n_r,$$

$$b_m^{\text{TE}}(k) = [n_r J'_m(x)J_m(n_r x) - J_m(x)J'_m(n_r x)]\pi ix/2n_r,$$

$$c_m^{\text{TE}}(k) = [n_r H'_m(x)H_m(n_r x) - H_m(x)H'_m(n_r x)]\pi in_r x/2$$

with x = kR. The Wronskian in the TM case is calculated to be

$$W^{\mathrm{TM}}(f_m, g_m) = 2ia_m(k)/\pi = -xD_m^{\mathrm{TM}}(x)$$

and in the TE case

$$W^{\mathrm{TE}}(f_m, g_m) = 2in_r^2 a_m(k) = -nx D_m^{\mathrm{TE}}(x)/\pi,$$

with $D_m^{\text{TM}}(x)$ defined in Eq. (4.25) and $D_m^{\text{TE}}(x)$ defined in Eq. (4.26). Inside the cylinder, the GF then takes the form

$$\tilde{G}_{m}(\rho,\rho';k) = \frac{\pi}{2i}\sqrt{\rho\rho'} \bigg[J_{m}(n_{r}k\rho_{<})H_{m}(n_{r}k\rho_{>}) + \frac{c_{m}(k)}{a_{m}(k)}J_{m}(n_{r}k\rho_{<})J_{m}(n_{r}k\rho_{>}) \bigg], \qquad (E.8)$$

using the TM (TE) version of $a_m(k)$ and $c_m(k)$ for the TM (TE) GF. The GF has simple poles k_n in the complex k-plane which are the wave vectors of RSs, given by $a_m(k_n) = 0$, an equation equivalent to Eq. (4.23). The residues Res_n of the GF at these poles are calculated for the TM modes using

$$r_m^{\rm TM}(k_n) = \frac{c_m^{\rm TM}(k)}{\frac{d}{dk} a_m^{\rm TM}(k)} \bigg|_{k=k_n} = \frac{2ik_n}{\pi (n_r^2 - 1)[k_n R J_m(n_r k_n R)]^2},$$
 (E.9)

and for the TM modes using

$$r_m^{\rm TE}(k_n) = -\frac{c_m^{\rm TE}(k)}{\frac{d}{dk}a_m^{\rm TE}(k)}\bigg|_{k=k_n} = \frac{2i}{\pi(n_r^2 - 1)\left[\frac{m^2}{k_n}\left[J_m(nk_nR)\right]^2 + R^2k_n\left[J_m'(nk_nR)\right]^2\right]}.$$
(E.10)

In addition to the poles, the GF has a cut in the complex k-plane along the negative imaginary half-axis. The cut is due to the Hankel function $H_m(z)$ which describes the field outside the cylinder and contributes to Eqs. (4.23), (4.24) and Eq. (E.8), and is not uniquely defined. Indeed, it can be expressed as [55]

$$H_m(z) = J_m(z) + iN_m(z),$$
 (E.11)

using a multiple-valued Neumann function

$$N_m(z) = \tilde{N}_m(z) + \frac{2}{\pi} J_m(z) \ln \frac{z}{2}, \qquad (E.12)$$

where $\tilde{N}_m(z) = z^m F_m(z^2)$ is a single-valued polynomial [55] while $\ln z$ is a multiplevalued function defined on an infinite number of Riemann sheets. We have verified that only one such sheet provides the asymptotics $H_m(z) \propto \exp(iz)/\sqrt{z}$ for $z \to \infty$, which is required for the RS wave functions outside the cylinder to satisfy the outgoing wave boundary conditions Eq. (2.7). This 'physical' sheet has a cut going from the branch point at z = 0 to infinity, and the position of this cut is not arbitrary. To find the cut position let use the symmetry of the RS wave numbers, $k_{-n} = -k_n^*$, discussed in Sec. 2.1. Let us also, using properties of cylindrical functions, [55] bring the secular equation (4.23) to the form

$$J_{m+1}(n_r z)H_{m-1}(z) = J_{m-1}(n_r z)H_{m+1}(z), \qquad (E.13)$$

in which $z = k_n R$. We note that if $z = k_n R$ is a complex solution of Eq. (E.13), then $-z^*$ is also a solution of the same equation. We take two equations, one is the conjugate of Eq. (E.13) and the other is Eq. (E.13) itself but taken with the argument $-z^*$, and add them up. Substituting there Eqs. (E.11) and (E.12) and using the facts that [55]

$$\begin{bmatrix} J_m(z) \end{bmatrix}^* = J_m(z^*) = (-1)^m J_m(-z^*) , \begin{bmatrix} \tilde{N}_m(z) \end{bmatrix}^* = \tilde{N}_m(z^*) = (-1)^m \tilde{N}_m(-z^*) ,$$

we arrive at the condition

$$\ln(-z^*) - (\ln z)^* = \pi i, \qquad (E.14)$$

which is fulfilled, for any z, only if $\ln z$ [and consequently $H_m(z)$] has a cut along the negative imaginary half-axis.

Owing to the cut of the Hankel function $H_m(z)$ the GF also has a cut along the negative imaginary half-axis in the complex k-plane, so that on both sides of the cut \tilde{G}_m takes different values: \tilde{G}_m^+ on the right-hand side and \tilde{G}_m^- on the left-hand side of the cut. The step $\Delta \tilde{G}_m = \tilde{G}_m^+ - \tilde{G}_m^-$ over the cut can be calculated using the corresponding difference in the Hankel function:

$$\Delta H_m(z) = H_m^+(z) - H_m^-(z) = 4J_m(z) \,.$$

The result is

$$\Delta \tilde{G}_m(\rho, \rho'; k) = \frac{\pi}{2i} \sqrt{\rho \rho'} J_m(n_r k \rho_<) J_m(n_r k \rho_>) \Delta Q_m(k)$$
(E.15)

where

$$\Delta Q_m(k) = \left[4 + \frac{c_m^+}{a_m^+} - \frac{c_m^-}{a_m^-}\right] = -\left(\frac{4}{\pi kR}\right)^2 \frac{1}{D_m^+(kR)D_m^-(kR)}$$
(E.16)

with $D_m(kR)$ given by Eq. (4.25) in the case of the GF for TM modes or Eq. (4.26) in the case of the GF for the TE modes.

Let us now use the residue theorem for the function $\tilde{G}_m(\rho, \rho'; k')/(k - k')$ integrating it in the complex k'-plane along a closed contour consisting of three parts,



Figure E.1: Sketch showing the contour of integration in Eq. (E.17) as well as poles (black dots) and the cut (blue dashed line) of the GF in the complex k'-plane. An extra pole at k' = k is shown by a red dot.

see Fig. E.1: A large counter-clockwise circumference with a radius tending to infinity, two straight lines circumventing the cut and approaching it from both sides, and a small clockwise circumference around the origin with a radius tending to zero. Since the GF behaves as k^{-2} at large values of k and takes finite values or logarithmically diverges at k = 0, both large- and small-circle integrals vanish, so that the only remaining integrals are those which are taken along the cut:

$$\oint \frac{\tilde{G}_m(\rho, \rho'; k')}{k - k'} dk' = \int_0^{-i\infty} \frac{\tilde{G}_m^+ dk'}{k - k'} + \int_{-i\infty}^0 \frac{\tilde{G}_m^- dk'}{k - k'} \\ = 2\pi i \sum_n \frac{\text{Res}_n}{k - k_n} - 2\pi i \tilde{G}_m(\rho, \rho'; k) \,.$$
(E.17)

Note that in the second part of the above equation we have made use of the residue theorem, expressing the closed-loop integral in the left-hand side in terms of a sum over residues at all poles inside the contour. Using Eq. (E.17) the GF can be expressed as

$$\tilde{G}_m(\rho,\rho';k) = \sum_n \frac{\operatorname{Res}_n}{k-k_n} + \frac{1}{2\pi i} \int_{-i\infty}^0 \frac{\Delta \tilde{G}_m(\rho,\rho';k')dk'}{k-k'}, \quad (E.18)$$

which is a generalization of the Mittag-Leffler theorem. This is used in Sec. 4.1 when applying the RSE to 2D systems with a cut their GF. The residues Res_n of the GF contributing to Eq. (E.18) are calculated as

$$\operatorname{Res}_{n} = \frac{\pi}{2i} \sqrt{\rho \rho'} J_{m}(n_{r} k \rho_{<}) J_{m}(n_{r} k \rho_{>}) r_{m}(k_{n}) , \qquad (E.19)$$

where we use $r_m(k_n)$ found in Eq. (E.9) for the TM modes or Eq. (E.10) for the TE modes. Given that the spatial dependence of the GF, as described by Eqs. (E.18), (E.19), and (E.15), is represented by products of the RS wave functions $R_m(\rho, k_n)$ and their analytic continuations $R_m(\rho, k)$ with k-values taken on the cut, we arrive at the GF in the form of Eqs. (4.33) and (B.13) which are then used in the RSE.

Appendix F

Matrix elements used in 2D RSE

In this section we give explicit expressions for the matrix elements $V_{\bar{n}\bar{n}'}$ of the specific perturbations considered in this paper. As a starting point we use the following general formula for the matrix elements of an arbitrary perturbation $\Delta \varepsilon(\rho, \varphi)$ inside the cylinder of radius R:

$$V_{nn'} = \int \mathbf{E}_n(\mathbf{r}) \Delta \hat{\boldsymbol{\varepsilon}}(\mathbf{r}) \mathbf{E}_m(\mathbf{r}) \, d\mathbf{r} \,, \tag{F.1}$$

in which R_m and χ_m are the eigenfunctions of the homogeneous cylinder given in Sec. 4.1.3.

F.1 Homogeneous cylinder perturbation for TM modes

The homogeneous scalar perturbation Eq. (5.17) does not mix different *m*-values or polarisations. The TM matrix elements between RS with the same azimuthal number *m* and TM polarisation are given by the radial overlap integrals

$$V_{\bar{n}\bar{n}'} = \Delta \epsilon \int_0^R R_m(\rho, k_{\bar{n}}) R_m(\rho, k_{\bar{n}'}) \rho d\rho$$
(F.2)
yielding for identical basis states $(\bar{n}=\bar{n}')$

$$V_{\bar{n}\bar{n}} = \frac{\Delta\epsilon}{n_r^2 - 1} \left[1 - \frac{J_{m-1}(n_r k_{\bar{n}} R) J_{m+1}(n_r k_{\bar{n}} R)}{[J_m(n_r k_{\bar{n}} R)]^2} \right]$$
(F.3)

and for different basis states $(\bar{n} \neq \bar{n}')$

$$V_{\bar{n}\bar{n}'} = \frac{\Delta\epsilon}{n_r^2 - 1} \frac{2}{n_r R(k_{\bar{n}}^2 - k_{\bar{n}'}^2)} \left[k_{\bar{n}'} \frac{J_{m-1}(n_r k_{\bar{n}'}R)}{J_m(n_r k_{\bar{n}'}R)} - k_{\bar{n}} \frac{J_{m-1}(n_r k_{\bar{n}}R)}{J_m(n_r k_{\bar{n}}R)} \right] .$$
(F.4)

F.2 Homogeneous cylinder perturbation for TE Modes

The homogeneous scalar perturbation Eq. (5.17) does not mix different *m*-values or polarisations. The matrix elements between RS with the same azimuthal number *m* and TE polarisation are given by the radial overlap integrals

$$V_{\bar{n}\bar{n}'} = \frac{A_m^{TE}(k_{\bar{n}})A_m^{TE}(k_{\bar{n}'})\gamma_m(k_{\bar{n}})\gamma_m(k_{\bar{n}'})\Delta\epsilon}{2} \left[I_{m-1}(k_{\bar{n}},k_{\bar{n}'}) + I_{m+1}(k_{\bar{n}},k_{\bar{n}'}) \right]$$
(F.5)

where $A_m^{TE}(k_{\bar{n}})$ is defined by Eq. (4.22) and

$$\gamma_m(k_{\bar{n}}) = \begin{cases} \sqrt{m(n_r^2 - 1)} & \text{for } k_{\bar{n}} = 0, \\ 1 & \text{otherwise} \end{cases}$$
(F.6)

$$I_{j}(k_{\bar{n}}, k_{\bar{n}'}) = \int_{R} J_{j}(nk_{\bar{n}}\rho') J_{j}(nk_{\bar{n}'}\rho')\rho' d\rho'$$
(F.7)

yielding for identical basis states $(\bar{n} = \bar{n}')$

$$I_m(k_{\bar{n}}, k_{\bar{n}'}) = \frac{R^2}{2} \left[\left[J_m(n_r k_{\bar{n}} R) \right]^2 - J_{m-1}(n_r k_{\bar{n}} R) J_{m+1}(n_r k_{\bar{n}} R) \right]$$
(F.8)

and for different basis states $(\bar{n} \neq \bar{n}')$

$$\frac{Rn_r}{k_{\bar{n}}^2 - k_{\bar{n}'}^2} k_{\bar{n}'} J_m(k_{\bar{n}} n_r R) J_{m-1}(k_{\bar{n}'} n_r R) - \frac{Rn_r}{k_{\bar{n}}^2 - k_{\bar{n}'}^2} k_{\bar{n}} J_m(k_{\bar{n}'} n_r R) J_{m-1}(k_{\bar{n}} n_r R) = I_m(k_{\bar{n}}, k_{\bar{n}'}) \quad (F.9)$$

When $k_{\bar{n}} = 0$ we can use the asymptotic form of the Bessel function,

$$J_m(z) = \frac{(z/2)^m}{m!}$$
(F.10)

from which we see if $k_{\bar{n}} \to 0$ then $k_{\bar{n}}$ cancels out everywhere in V_{nm} .

F.3 HALF-CYLINDER PERTURBATION FOR TM MODES

The most efficient way of calculating the TM matrix elements of the perturbation Eq. (4.39) is to calculate the angular parts of the integrals analytically and the radial parts numerically. The matrix elements have the form

$$V_{\bar{n}\bar{n}} = \Delta \epsilon P_{mm'} Q_{k_{\bar{n}}k_{\bar{n}'}}^{mm'}, \qquad (F.11)$$

in which the angular overlap integrals $P_{mm'}$ are vanishing when taken between modes of different parity, i.e. between sine and cosine modes, and between same parity modes corresponding to azimuthal numbers m and m' of different parity. The non-vanishing integrals are given by

$$P_{mm'} = \int_{-\pi/2}^{\pi/2} \chi_m(\varphi) \chi_{m'}(\varphi) d\varphi - \int_{\pi/2}^{3\pi/2} \chi_m(\varphi) \chi_{m'}(\varphi) d\varphi$$
$$= s_m s_{m'}(\psi_{m-m'} \pm \psi_{m+m'})$$
(F.12)

with +(-) corresponding to cosine (sine) modes and s_m and ψ_m defined as

$$s_m = \begin{cases} \pi^{-1/2} & \text{for } m \neq 0, \\ (2\pi)^{-1/2} & \text{for } m = 0, \end{cases}$$
$$\psi_m = \left[1 - (-1)^m\right] \frac{\sin(m\pi/2)}{m}.$$

The radial part of the matrix elements of the perturbation is given by the integrals

$$Q_{kk'}^{mm'} = \int_{0}^{R} R_{m}(\rho, k) R_{m'}(\rho, k') \rho d\rho$$

$$= \frac{2}{R^{2}(n_{r}^{2} - 1)} \frac{\int_{0}^{R} J_{m}(n_{r}k\rho) J_{m'}(n_{r}k'\rho) \rho d\rho}{J_{m}(n_{r}kR) J_{m'}(n_{r}k'R)}$$
(F.13)

which we calculate numerically.

F.4 THIN-FILM PERTURBATION OF TM MODES

The TM matrix elements of the perturbation Eq. (4.40) are given by the integrals

$$V_{\bar{n}\bar{n}'} = h\Delta\epsilon\chi_m^2(0)\int_0^R R_m(\rho, k_{\bar{n}})R_{m'}(\rho, k_{\bar{n}'})d\rho, \qquad (F.14)$$

similar to Eq. (F.13), which are calculated numerically.

F.5 Thin-wire perturbation of TM modes

The RSE perturbation TM matrix elements for this system are calculated by summing I same-strength delta scatterers on a square grid covering a circle. The perturbation Eq. (4.41) is thus modeled by

$$\Delta \varepsilon \approx \Delta \epsilon \frac{\pi b^2}{I} \sum_{i=1}^{I} \frac{1}{\rho} \delta(\rho - \rho_i) \delta(\varphi - \varphi_i) \,. \tag{F.15}$$

The matrix elements then have the form

$$V_{\bar{n}\bar{n}'} = \Delta \epsilon \frac{\pi b^2}{I} \sum_{i=1}^{I} E_{\bar{n}}(\rho_i, \varphi_i) E_{\bar{n}'}(\rho_i, \varphi_i)$$
(F.16)

with $E_{\bar{n}}(\rho,\varphi)$ given by Eq. (4.28).

Appendix G

Matrix Elements used in the 3D RSE

In this section we give the matrix elements required to reproduce the numerical results of Chapter 5.

G.1 Homogeneous sphere perturbation

The homogeneous perturbation Eq. (5.17) does not mix different m or l values, nor does it mix TE modes with TM or L modes. Using the definition Eq. (2.36) we calculate the matrix elements between TE RSs performing the angular integration which leads to the lm-orthogonality:

$$V_{nn'}^{\rm TE} = \Delta \epsilon \, l(l+1) \delta_{ll'} \delta_{mm'} (A_l^{\rm TE})^2 \int_0^R R_l(r,k_n) R_l(r,k_{n'}) r^2 dr.$$

The radial integration can also be done analytically, so that the matrix elements take the form

$$V_{nn}^{\rm TE} = \frac{\Delta \epsilon}{n_r^2 - 1} \left[1 - \frac{j_{l-1}(x)j_{l-1}(x)}{j_l^2(x)} \right]$$
(G.1)

for identical basis states n = n' and

$$V_{nn'}^{\rm TE} = \frac{\Delta \epsilon}{n_r^2 - 1} \frac{2\delta_{ll'}\delta_{mm'}}{x^2 - y^2} \left[\frac{yj_{l-1}(y)}{j_l(y)} - \frac{xj_{l-1}(x)}{j_l(x)} \right]$$
(G.2)

for different basis states $n \neq n'$, where $x = n_r k_n R$ and $y = n_r k_{n'} R$.

Similarly, for TM RSs have

$$V_{nn'}^{\mathrm{TM}} = \frac{\Delta \epsilon \, l(l+1)}{n_r^4 k_n k_{n'}} \delta_{ll'} \delta_{mm'} A_l^{\mathrm{TM}}(k_n) A_l^{\mathrm{TM}}(k_{n'}) \\ \times \int_0^R \left\{ l(l+1) R_l(r,k_n) R_l(r,k_{n'}) \\ + \frac{\partial [r R_l(r,k_n)]}{\partial r} \frac{\partial [r R_l(r,k_{n'})]}{\partial r} \right\} dr \,,$$

and performing analytic integration obtain

$$V_{nn}^{\rm TM} = \frac{\Delta \epsilon}{n_r^2 - 1} \frac{1}{F_l(x)} \left[2\frac{l+1}{x^2} + \frac{j_{l+1}^2(x)}{j_l^2(x)} - \frac{j_{l+2}(x)}{j_l(x)} \right]$$
(G.3)

for identical basis states n = n' and

$$V_{nn'}^{\text{TM}} = \frac{\Delta \epsilon}{n_r^2 - 1} \frac{1}{\sqrt{F_l(x)F_l(y)}} \frac{2\delta_{ll'}\delta_{mm'}}{x^2 - y^2}$$

$$\times \left[(x^2 - y^2)\frac{l+1}{xy} + \frac{yj_{l+1}(x)}{j_l(x)} - \frac{xj_{l+1}(y)}{j_l(y)} \right]$$
(G.4)

for different basis states $n \neq n'$, where

$$F_l(x) = \left[\frac{j_{l-1}(x)}{j_l(x)} - \frac{l}{x}\right]^2 + \frac{n_r^2 l(l+1)}{x^2}, \qquad (G.5)$$

 $x = n_r k_n R$, and $y = n_r k_{n'} R$.

Note that L and TM modes are mixed by the perturbation, and non-vanishing matrix elements between them are calculated using Eqs. (G.3) and (G.4), treating the L modes as TM modes with $k_n = 0$ and the normalization constants multiplied by $\sqrt{l(n_r^2 - 1)}$, in accordance with Eq. (5.16).

G.2 Arbitrary perturbations

An arbitrary perturbation of the sphere can be treated as a superposition of homogeneous perturbations in the form of spherical-shell pieces, each piece described by

$$\Delta \varepsilon(\mathbf{r}) = \begin{cases} R_1 \leqslant r \leqslant R_2 \\ \Delta \epsilon & \text{for} \quad \theta_1 \leqslant \theta \leqslant \theta_2 \\ \varphi_1 \leqslant \varphi \leqslant \varphi_2 \\ 0 & \text{otherwise.} \end{cases}$$
(G.6)

The hemisphere perturbations like Eq. (5.18) are then described by Eq. (G.6) with $0 \leq r \leq R$, $0 \leq \theta \leq \pi/2$ $(\pi/2 \leq \theta \leq \pi)$, and $0 \leq \varphi \leq 2\pi$. The quarter sphere perturbation Eq. (5.19) is given by Eq. (G.6) with $0 \leq r \leq R$, $0 \leq \theta \leq \pi/2$, and $\pi/2 \leq \varphi \leq 3\pi/2$.

Factorizing the radial and angular integrals, the matrix elements of the perturbations Eq. (G.6) become

$$V_{nn'}^{\text{TE}} = \Delta \epsilon A_l^{\text{TE}} A_{l'}^{\text{TE}}$$

$$\times T_{1;nn'}^{ll'} \left(mm' S_{-m}^{-m'} Q_{1;ll'}^{mm'} + S_m^{m'} Q_{2;ll'}^{mm'} \right)$$
(G.7)

between TE modes,

$$V_{nn'}^{\rm TM} = \Delta \epsilon \frac{A_l^{\rm TM}(k_n) A_{l'}^{\rm TM}(k_{n'})}{n_r^4 k_n k_{n'}} \left[l^2 (l+1)^2 T_{2;nn'}^{ll'} S_m^{m'} Q_{3;ll'}^{mm'} + T_{3;nn'}^{ll'} \left(mm' S_{-m}^{-m'} Q_{1;ll'}^{mm'} + S_m^{m'} Q_{2;ll'}^{mm'} \right) \right]$$
(G.8)

between TM (including L) modes, and

$$V_{nn'}^{\text{TE-TM}} = \Delta \epsilon A_l^{\text{TE}} \frac{A_{l'}^{\text{TM}}(k_{n'})}{n_r^2 k_{n'}}$$

$$\times T_{4;nn'}^{ll'} \left(m S_{-m}^{m'} Q_{4;ll'}^{mm'} - m' S_m^{-m'} Q_{4;l'l}^{m'm} \right)$$
(G.9)

between TE and TM (including L) modes. The integrals contributing to Eqs. (G.7),

(G.8), and (G.9) are given by

$$\begin{split} T_{1;nn'}^{ll'} &= \int_{R_1}^{R_2} r^2 dr \bar{j}_l(n_r k_n r) \bar{j}_{l'}(n_r k_n' r) \\ T_{2;nn'}^{ll'} &= \int_{R_1}^{R_2} dr \bar{j}_l(n_r k_n r) \bar{j}_{l'}(n_r k_n' r) \\ T_{3;nn'}^{ll'} &= \int_{R_1}^{R_2} dr \frac{d}{dr} \Big[\bar{j}_l(n_r k_n r) \Big] \frac{d}{dr} \Big[\bar{j}_{l'}(n_r k_n' r) \Big] \\ T_{4;nn'}^{ll'} &= \int_{R_1}^{R_2} r dr \bar{j}_l(n_r k_n r) \frac{d}{dr} \Big[\bar{j}_{l'}(n_r k_n' r) \Big] \\ S_m^{m'} &= \int_{\varphi_1}^{\varphi_2} d\varphi \chi_m(\varphi) \chi_{m'}(\varphi) \\ Q_{1;ll'}^{nm'} &= \int_{\theta_1}^{\theta_2} d\theta \frac{\bar{P}_l^m(\cos \theta) \bar{P}_{l'}^{m'}(\cos \theta)}{\sin \theta} \\ Q_{2;ll'}^{nm'} &= \int_{\theta_1}^{\theta_2} \sin \theta d\theta \frac{d}{d\theta} \Big[\bar{P}_l^m(\cos \theta) \Big] \frac{d}{d\theta} \Big[\bar{P}_{l'}^{m'}(\cos \theta) \Big] \\ Q_{3;ll'}^{nm'} &= \int_{\theta_1}^{\theta_2} \sin \theta d\theta \bar{P}_l^m(\cos \theta) \bar{P}_{l'}^{m'}(\cos \theta) \\ Q_{4;ll'}^{nm'} &= \int_{\theta_1}^{\theta_2} d\theta \bar{P}_l^m(\cos \theta) \frac{d}{d\theta} \Big[\bar{P}_{l'}^{m'}(\cos \theta) \Big] , \end{split}$$
(G.10)

where

$$\bar{j}_l(kr) \equiv \frac{j_l(kr)}{j_l(kR)} \tag{G.11}$$

and

$$\bar{P}_{l}^{m}(x) \equiv \sqrt{\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}} P_{l}^{|m|}(x) \,. \tag{G.12}$$

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